

Support Information

Refining Details of the Structural and Electronic Properties of the Cu_B Site in pMMO Enzyme through Sequential Molecular Dynamics/CPKS-EPR Calculations.

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1 - PropKa Protonation States of the Amino Acid Residues.

The pKa calculated using PropKa¹ were used mainly to decide, together with careful analysis, the protonation states of the residues that compose the first coordination sphere (HIS³³, HIS¹³⁷, HIS¹³⁹) around the copper ion in the Cu_B site plus the GLU³⁵. In addition, residues whose calculated pKa values differed considerably from the predicted model also were analyzed individually, for instance, the residues ASP⁵¹, ASP³³², HIS⁴⁸, and GLU⁷⁵.

PropKa Output

RESIDUE	pKa	LOCATE	DESOLVATION MASSIVE	EFFECTS LOCAL	SIDECCHAIN HYDROGEN BOND	BACKBONE HYDROGEN BOND	COULOMBIC INTERACTION
GLU 35	4.77	BURIED	1.04 504	0.63 9	0.00 000 0	-0.31 HIS 33	0.00 000 0
GLU 35					0.00 000 0	-1.09 GLU 35	0.00 000 0
ASP 51	-0.74	BURIED	1.15 515	0.56 8	-0.67 LYS 70	0.00 000 0	-2.37 LYS 70
ASP 51					-0.80 ARG 400	0.00 000 0	-2.40 ARG 400
GLU 57	3.88	SUFACE	0.00 317	0.14 2	-0.76 LYS 155	0.00 000 0	0.00 000 0
GLU 63	3.15	SUFACE	0.00 283	0.28 4	-0.48 LYS 56	-1.14 LYS 60	0.00 000 0
GLU 66	3.44	SUFACE	0.00 339	0.42 6	-0.78 LYS 68	0.00 000 0	0.00 000 0
GLU 66					-0.70 ARG 125	0.00 000 0	0.00 000 0
GLU 75	0.08	BURIED	0.65 465	0.77 11	-0.80 GLN 404	-1.04 GLU 75	-2.40 HIS 72
GLU 75					-1.60 HIS 72	0.00 000 0	0.00 000 0
GLU 79	4.57	SUFACE	0.00 160	0.07 1	0.00 000 0	0.00 000 0	0.00 000 0
ASP 82	3.93	SUFACE	0.00 223	0.14 2	0.00 000 0	-0.01 ASP 82	0.00 000 0
GLU 83	4.50	SUFACE	0.00 267	0.00 0	0.00 000 0	0.00 000 0	0.00 000 0
ASP 85	3.72	SUFACE	0.00 288	0.35 5	-0.43 ARG 115	0.00 000 0	0.00 000 0
GLU 102	3.78	SUFACE	0.00 315	0.28 4	-0.65 TYR 104	0.00 000 0	0.00 000 0
GLU 102					-0.35 ARG 125	0.00 000 0	0.00 000 0
GLU 117	4.12	SUFACE	0.00 296	0.14 2	-0.52 ARG 115	0.00 000 0	0.00 000 0
ASP 123	3.34	SUFACE	0.00 385	0.35 5	0.00 000 0	-0.20 GLY 106	0.00 000 0
ASP 123					0.00 000 0	-0.61 ASP 123	0.00 000 0
ASP 135	3.35	SUFACE	0.00 286	0.35 5	-0.80 THR 158	0.00 000 0	0.00 000 0
GLU 160	3.89	SUFACE	0.00 198	0.07 1	-0.68 LYS 58	0.00 000 0	0.00 000 0
GLU 165	4.50	SUFACE	0.00 180	0.00 0	0.00 000 0	0.00 000 0	0.00 000 0
ASP 179	2.64	SUFACE	0.00 256	0.98 14	0.00 000 0	-0.99 ASN 168	0.00 000 0

ASP 179								0.00 000 0	-1.15 GLU 181	0.00 000 0		
GLU 181	4.12	SUFACE	0.00	300	0.42	6	-0.80 ARG 131	0.00 000 0	0.00 000 0	0.00 000 0		
GLU 276	4.64	SUFACE	0.00	206	0.14	2	0.00 000 0	0.00 000 0	0.00 000 0	0.00 000 0		
GLU 287	3.83	SUFACE	0.00	247	0.14	2	-0.80 THR 303	-0.01 GLU 287	0.00 000 0	0.00 000 0		
ASP 288	3.87	SUFACE	0.00	270	0.07	1	0.00 000 0	0.00 000 0	0.00 000 0	0.00 000 0		
GLU 316	4.13	BURIED	2.20	620	0.63	9	-0.80 ARG 323	0.00 000 0	-2.40 ARG 323			
ASP 326	2.50	SUFACE	0.00	399	0.77	11	-0.63 ASN 351	-0.91 ASP 328	0.00 000 0	0.00 000 0		
ASP 326							-0.73 ASP 328	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 326							0.20 ASP 344	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 328	4.53	SUFACE	0.00	266	0.21	3	0.73 ASP 326	-0.20 ASP 328	0.00 000 0	0.00 000 0		
ASP 332	-0.05	BURIED	0.43	443	1.12	16	-0.80 THR 334	-0.12 THR 333	-1.95 ARG 323			
ASP 332							-0.78 ARG 323	-0.48 THR 334	0.00 000 0	0.00 000 0		
ASP 332							0.00 000 0	-0.29 GLY 335	0.00 000 0	0.00 000 0		
ASP 332							0.00 000 0	-0.99 TYR 336	0.00 000 0	0.00 000 0		
GLU 338	5.24	SUFACE	0.00	311	0.21	3	0.53 GLU 343	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 339	2.14	BURIED	0.49	449	0.35	5	-0.80 TYR 374	-0.60 ASP 339	-1.08 HIS 137			
ASP 339							0.00 000 0	-0.02 LEU 340	0.00 000 0	0.00 000 0		
GLU 343	3.70	SUFACE	0.00	313	0.35	5	-0.53 GLU 338	-0.62 GLU 343	0.00 000 0	0.00 000 0		
ASP 344	2.02	SUFACE	0.00	314	0.49	7	-0.80 SER 327	-1.11 SER 327	0.00 000 0	0.00 000 0		
ASP 344							-0.20 ASP 326	-0.16 ASP 328	0.00 000 0	0.00 000 0		
ASP 350	2.26	SUFACE	0.00	293	0.63	9	-0.80 SER 352	-1.13 SER 352	0.00 000 0	0.00 000 0		
ASP 350							-0.23 ARG 360	0.00 000 0	0.00 000 0	0.00 000 0		
GLU 358	4.11	SUFACE	0.00	217	0.07	1	-0.10 ARG 360	-0.35 ALA 355	0.00 000 0	0.00 000 0		
ASP 363	3.52	SUFACE	0.00	306	0.42	6	-0.23 LYS 301	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 363							-0.48 ARG 299	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 368	3.00	SUFACE	0.00	393	0.42	6	0.00 000 0	-0.02 ALA 369	0.00 000 0	0.00 000 0		
ASP 368							0.00 000 0	-1.19 ALA 370	0.00 000 0	0.00 000 0		
GLU 372	4.71	SUFACE	0.00	273	0.21	3	0.00 000 0	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 378	3.56	SUFACE	0.00	334	0.56	8	-0.80 ARG 375	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 382	4.56	BURIED	0.42	442	1.05	15	0.00 000 0	-0.15 ALA 40	0.00 000 0	0.00 000 0		
ASP 382							0.00 000 0	-0.57 PHE 41	0.00 000 0	0.00 000 0		
ASP 384	1.82	SUFACE	0.00	342	0.42	6	-2.40 ARG 386	0.00 000 0	0.00 000 0	0.00 000 0		
ASP 395	2.60	SUFACE	0.00	285	0.98	14	-0.32 SER 310	-0.12 ASP 395	0.00 000 0	0.00 000 0		
ASP 395							-0.45 THR 397	-0.19 THR 397	0.00 000 0	0.00 000 0		
ASP 395							0.00 000 0	-0.12 GLY 398	0.00 000 0	0.00 000 0		
ASP 395							0.00 000 0	-0.98 ASN 399	0.00 000 0	0.00 000 0		
ASP 406	1.66	BURIED	0.31	431	0.35	5	-0.80 ARG 45	0.00 000 0	-2.00 ARG 45			
HIS 33	6.50	SUFACE	0.00	348	-0.00	0	0.00 000 0	0.00 000 0	0.00 000 0	0.00 000 0		
HIS 48	1.04	BURIED	-2.51	651	-3.29	47	0.01 GLN 404	1.10 MET 44	-0.77 HIS 72			
HIS 48							0.00 000 0	0.00 ALA 388	0.00 000 0	0.00 000 0		
HIS 72	6.92	BURIED	-1.57	557	-2.73	39	1.60 GLU 75	0.72 GLY 119	2.40 GLU 75			
HIS 137	4.65	BURIED	-0.65	465	-2.73	39	0.00 000 0	0.45 GLY 154	1.08 ASP 339			

HIS 139	0.36	BURIED	-1.50	550	-3.08	44	0.00	000	0	0.00	000	0	-1.56	HIS 137
HIS 307	6.50	SUFACE	0.00	206	-0.00	0	0.00	000	0	0.00	000	0	0.00	000 0
TYR 50	10.89	BURIED	1.37	537	0.00	0	-0.11	THR 121	0.00	000	0	0.92	ASP 51	
TYR 50							0.00	000 0	0.00	000	0	-0.44	ARG 400	
TYR 50							0.00	000 0	0.00	000	0	-0.84	LYS 70	
TYR 104	13.03	SUFACE	0.00	275	0.07	1	0.65	GLU 102	0.00	000	0	2.40	GLU 102	
TYR 104							-0.09	ARG 125	0.00	000	0	0.00	000 0	
TYR 122	10.27	BURIED	0.56	456	0.07	1	0.00	000 0	-1.10	GLU 117	0.75	GLU 117		
TYR 183	9.70	SUFACE	0.00	188	0.00	0	-0.30	GLN 176	0.00	000	0	0.00	000 0	
TYR 258	10.00	SUFACE	0.00	151	0.00	0	0.00	000 0	0.00	000	0	0.00	000 0	
TYR 291	9.95	BURIED	0.05	405	0.35	5	-0.45	SER 385	0.00	000	0	0.00	000 0	
TYR 318	11.60	BURIED	3.66	766	0.21	3	-0.37	SER 321	-1.19	TRP 49	0.00	000 0		
TYR 318							0.00	000 0	-0.71	SER 321	0.00	000 0		
TYR 330	9.68	BURIED	0.49	449	0.00	0	-0.51	ARG 323	-0.05	THR 333	0.83	GLU 316		
TYR 330							0.00	000 0	0.00	000 0	0.88	ASP 332		
TYR 330							0.00	000 0	0.00	000 0	-1.58	ARG 323		
TYR 330							0.00	000 0	0.00	000 0	-0.39	ARG 400		
TYR 336	13.99	BURIED	2.93	693	0.21	3	0.00	000 0	0.00	000 0	-0.60	ARG 323		
TYR 336							0.00	000 0	0.00	000 0	1.45	TYR 318		
TYR 374	15.89	BURIED	0.85	485	0.07	1	0.80	ASP 339	0.00	000 0	1.77	GLU 35		
TYR 374							0.00	000 0	0.00	000 0	2.40	ASP 339		
TYR 381	11.09	SUFACE	0.00	228	0.00	0	0.00	000 0	0.00	000 0	1.09	ASP 378		
N+ 36	7.72	SUFACE	0.00	347	-0.28	4	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 56	10.15	SUFACE	0.00	285	-0.35	5	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 58	10.36	SUFACE	0.00	180	-0.14	2	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 60	10.50	SUFACE	0.00	177	-0.00	0	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 68	10.36	SUFACE	0.00	307	-0.14	2	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 70	12.59	BURIED	-0.48	448	-0.21	3	0.00	000 0	0.00	000 0	2.37	ASP 51		
LYS 70							0.00	000 0	0.00	000 0	0.84	TYR 50		
LYS 70							0.00	000 0	0.00	000 0	-0.43	ARG 400		
LYS 101	10.29	SUFACE	0.00	347	-0.21	3	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 120	10.50	SUFACE	0.00	270	-0.00	0	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 129	10.15	SUFACE	0.00	347	-0.35	5	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 155	9.73	BURIED	-0.21	421	-0.56	8	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 257	10.43	SUFACE	0.00	119	-0.07	1	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 273	10.50	SUFACE	0.00	183	-0.00	0	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 285	10.43	SUFACE	0.00	228	-0.07	1	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 301	10.29	SUFACE	0.00	246	-0.21	3	0.00	000 0	0.00	000 0	0.00	000 0		
LYS 331	10.29	SUFACE	0.00	225	-0.21	3	0.00	000 0	0.00	000 0	0.00	000 0		

ARG 43	9.85	BURIED	-1.60	560	-1.05	15	0.00 000	0	0.00 000	0	0.00 000	0
ARG 45	12.39	BURIED	-0.64	464	-1.47	21	0.00 000	0	0.00 000	0	2.00 ASP	406
ARG 100	10.95	BURIED	-0.85	485	-0.70	10	0.00 000	0	0.00 000	0	0.00 000	0
ARG 112	11.73	SUFACE	0.00	212	-0.77	11	0.00 000	0	0.00 000	0	0.00 000	0
ARG 115	11.66	SUFACE	0.00	268	-0.84	12	0.00 000	0	0.00 000	0	0.00 000	0
ARG 125	11.87	SUFACE	0.00	313	-0.63	9	0.00 000	0	0.00 000	0	0.00 000	0
ARG 131	11.94	SUFACE	0.00	327	-0.56	8	0.00 000	0	0.00 000	0	0.00 000	0
ARG 132	12.22	SUFACE	0.00	263	-0.28	4	0.00 000	0	0.00 000	0	0.00 000	0
ARG 167	12.08	SUFACE	0.00	205	-0.42	6	0.00 000	0	0.00 000	0	0.00 000	0
ARG 270	12.15	SUFACE	0.00	187	-0.35	5	0.00 000	0	0.00 000	0	0.00 000	0
ARG 292	11.73	SUFACE	0.00	195	-0.77	11	0.00 000	0	0.00 000	0	0.00 000	0
ARG 296	12.36	SUFACE	0.00	245	-0.14	2	0.00 000	0	0.00 000	0	0.00 000	0
ARG 299	12.36	SUFACE	0.00	316	-0.14	2	0.00 000	0	0.00 000	0	0.00 000	0
ARG 313	11.94	SUFACE	0.00	336	-0.56	8	0.00 000	0	0.00 000	0	0.00 000	0
ARG 323	16.49	BURIED	-1.56	556	-0.98	14	0.00 000	0	0.00 000	0	2.40 GLU	316
ARG 323							0.00 000	0	0.00 000	0	1.95 ASP	332
ARG 323							0.00 000	0	0.00 000	0	1.58 TYR	330
ARG 323							0.00 000	0	0.00 000	0	0.60 TYR	336
ARG 360	11.31	SUFACE	0.00	338	-1.19	17	0.00 000	0	0.00 000	0	0.00 000	0
ARG 375	12.29	SUFACE	0.00	278	-0.21	3	0.00 000	0	0.00 000	0	0.00 000	0
ARG 386	12.01	SUFACE	0.00	336	-0.49	7	0.00 000	0	0.00 000	0	0.00 000	0
ARG 400	14.16	BURIED	-1.01	501	-0.56	8	0.00 000	0	0.00 000	0	2.40 ASP	51
ARG 400							0.00 000	0	0.00 000	0	0.44 TYR	50
ARG 400							0.00 000	0	0.00 000	0	0.39 TYR	330

SUMMARY OF THIS PREDICTION

RESIDUE	pKa	pKmodel
ASP 51A	-0.74	3.80
ASP 82A	3.93	3.80
ASP 85A	3.72	3.80
ASP 123A	3.34	3.80
ASP 135A	3.35	3.80
ASP 179A	2.64	3.80
ASP 288A	3.87	3.80
ASP 326A	2.50	3.80
ASP 328A	4.53	3.80
ASP 332A	-0.05	3.80
ASP 339A	2.14	3.80
ASP 344A	2.02	3.80
ASP 350A	2.26	3.80
ASP 363A	3.52	3.80
ASP 368A	3.00	3.80
ASP 378A	3.56	3.80
ASP 382A	4.56	3.80

ASP	384A	1.82	3.80
ASP	395A	2.60	3.80
ASP	406A	1.66	3.80
GLU	35A	4.77	4.50
GLU	57A	3.88	4.50
GLU	63A	3.15	4.50
GLU	66A	3.44	4.50
GLU	75A	0.08	4.50
GLU	79A	4.57	4.50
GLU	83A	4.50	4.50
GLU	102A	3.78	4.50
GLU	117A	4.12	4.50
GLU	160A	3.89	4.50
GLU	165A	4.50	4.50
GLU	181A	4.12	4.50
GLU	276A	4.64	4.50
GLU	287A	3.83	4.50
GLU	316A	4.13	4.50
GLU	338A	5.24	4.50
GLU	343A	3.70	4.50
GLU	358A	4.11	4.50
GLU	372A	4.71	4.50
HIS	33A	6.50	6.50
HIS	48A	1.04	6.50
HIS	72A	6.92	6.50
HIS	137A	4.65	6.50
HIS	139A	0.36	6.50
HIS	307A	6.50	6.50
TYR	50A	10.89	10.00
TYR	104A	13.03	10.00
TYR	122A	10.27	10.00
TYR	183A	9.70	10.00
TYR	258A	10.00	10.00
TYR	291A	9.95	10.00
TYR	318A	11.60	10.00
TYR	330A	9.68	10.00
TYR	336A	13.99	10.00
TYR	374A	15.89	10.00
TYR	381A	11.09	10.00
N+	36A	7.72	8.00
LYS	56A	10.15	10.50
LYS	58A	10.36	10.50
LYS	60A	10.50	10.50
LYS	68A	10.36	10.50
LYS	70A	12.59	10.50
LYS	101A	10.29	10.50
LYS	120A	10.50	10.50
LYS	129A	10.15	10.50
LYS	155A	9.73	10.50
LYS	257A	10.43	10.50
LYS	273A	10.50	10.50
LYS	285A	10.43	10.50
LYS	301A	10.29	10.50
LYS	331A	10.29	10.50
ARG	43A	9.85	12.50
ARG	45A	12.39	12.50
ARG	100A	10.95	12.50
ARG	112A	11.73	12.50

ARG 115A	11.66	12.50
ARG 125A	11.87	12.50
ARG 131A	11.94	12.50
ARG 132A	12.22	12.50
ARG 167A	12.08	12.50
ARG 270A	12.15	12.50
ARG 292A	11.73	12.50
ARG 296A	12.36	12.50
ARG 299A	12.36	12.50
ARG 313A	11.94	12.50
ARG 323A	16.49	12.50
ARG 360A	11.31	12.50
ARG 375A	12.29	12.50
ARG 386A	12.01	12.50
ARG 400A	14.16	12.50

2 – Original RMSF of All Amino Acid Residues

Figure S1 present the original RMSF calculated from the 500 ns MD trajectory using the x-ray structure as reference. In the simulated model (only the soluble part) the alpha helices, originally bound to membrane, were taken off. This part of the protein is formed by the residues 185 to 256. Thus, the residues sequence in our model was renumbered from the residue 184. The RMSF in Figure S1 is in accordance with this renumeration. However, in the Figure 3 in main text of the manuscript, when necessary was performed the correspondence with the original sequence enumeration according with the 3RGB² file.

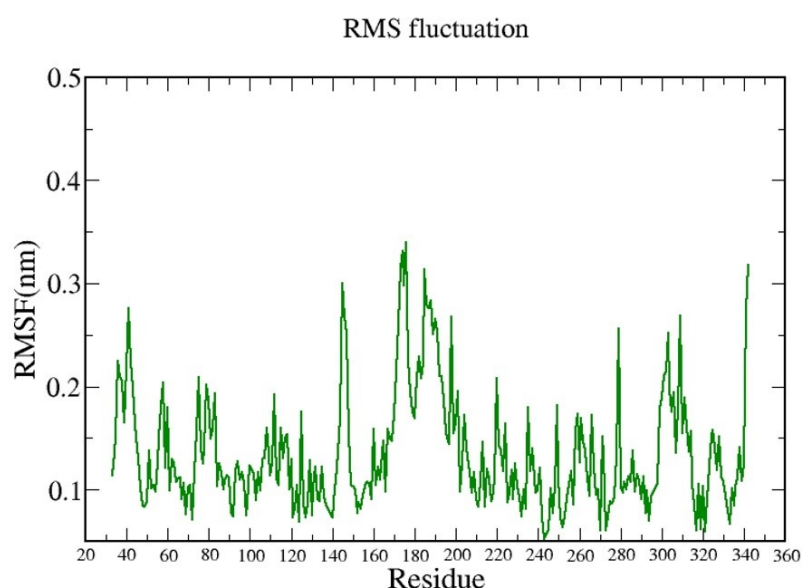


Figure S1: RMSF per residue of the 500 ns MD simulation of the soluble part of the pMMO.

Figure S2 shows the number of water molecules within a radius of 3 Å from Cu²⁺ ion in the Cu_B site.

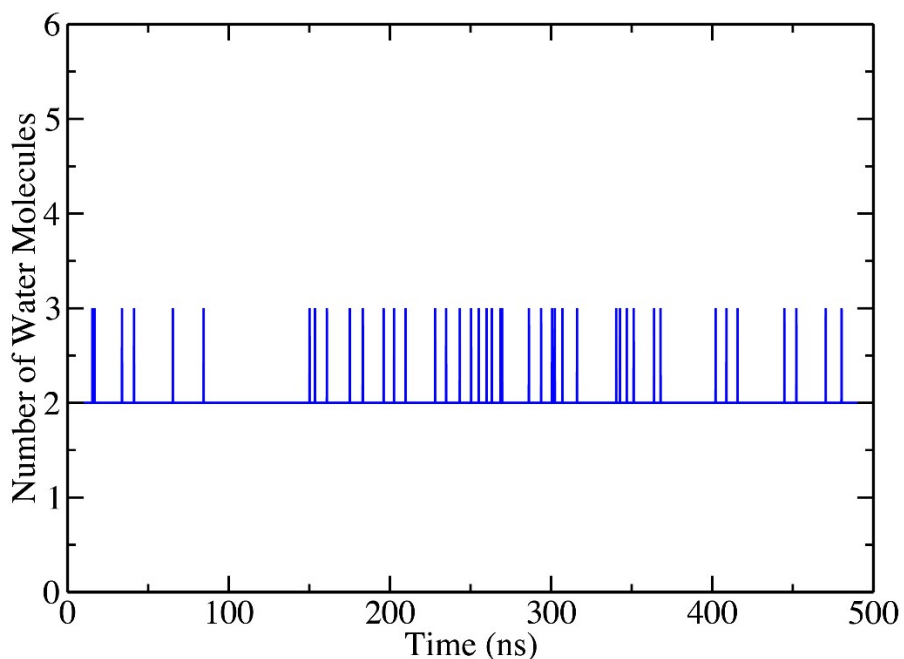


Figure S2: The number of water molecules within a radius of 6 Å from Cu²⁺ ion in the Cu_B site.

As shown in Figure S2, the number of water molecules within a radius of 3 Å from copper ion varies between 2 and 3, but with a significant occurrence in the average value of two molecules.

3 - LINCS Constraint

All bonds (C-H, N-H, O-H, S-H, C-C, C-N, C-O, C-S) were constrained according to the LINCS method.^{3,4} The expansion order of the constraint coupling matrix was 6. For the production NpT run, the number of iterations to correct for rotational lengthening was 1. In addition, the maximum angle of 30 degrees was defined as a criterion for that a bond can rotate before the LINCS algorithm gives a warning.

3 - Principal Component Analysis of the MD Simulation

To justify the statistical relevance of the snapshots used in the EPR parameters calculations, a PCA analysis⁵ was performed on the final 100 ns MD trajectory exploring different stages of the last 100 ns of the MD simulation trajectory. Figure S3 shows the eigenvalues calculated from the diagonalization of the covariance matrix of the backbone atoms fluctuations in function of the corresponding eigenvectors indexes. This analysis was carried out considering five conditions: (1) entire trajectory contained in the last 100 ns MD simulation, (2) every one nanosecond, (3) every two nanoseconds, (4) every five nanoseconds, and (5) frames saved every 10 ns.

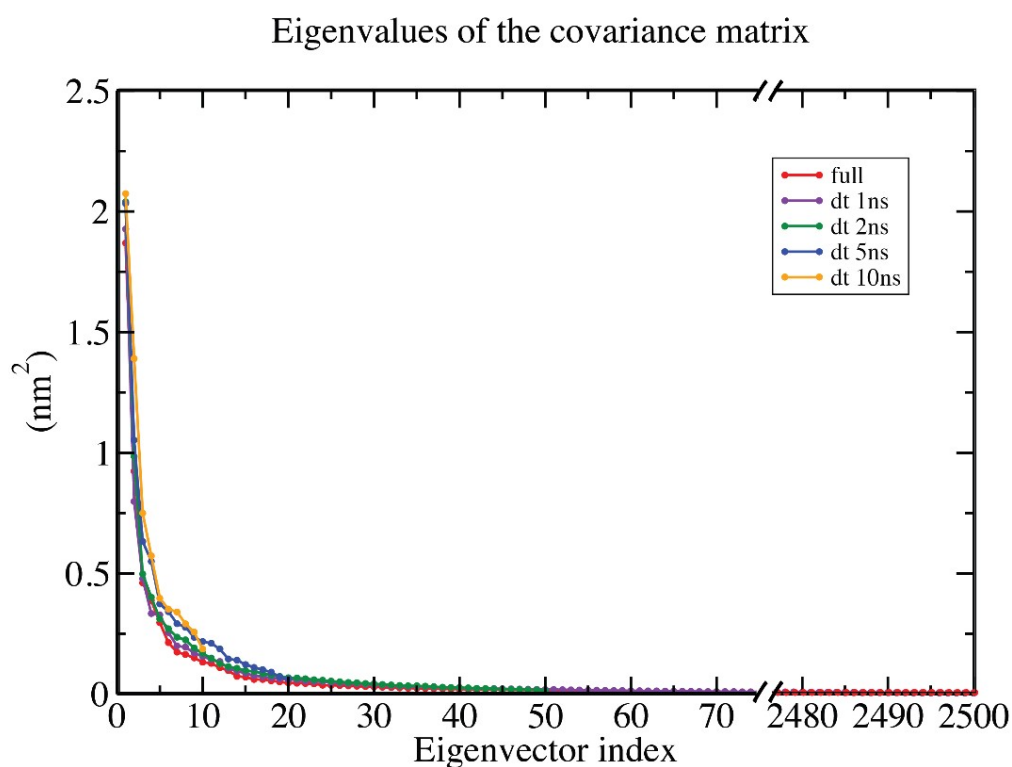


Figure S3: Plot of the eigenvalues against the corresponding eigenvector index calculated from diagonalization of the backbone atoms covariance matrix built from the last 100 ns MD trajectory of the 500 ns MD simulation.

As can be seen, the profiles are pretty similar for the five conditions analyzed. For all cases, the first five eigenvectors carry approximately more than 60 % of the total protein backbone motion of the simulated system, and the first 10 eigenvectors represent more than 80%. Table S1

shows the cumulative normalized eigenvalues for the first 20 modes corresponding to the condition (4) (every 5 nanoseconds). Also, it is possible to note in Figure S3 that after the eigenvector 20, the covariance practically does not change. The trace of the covariance matrix calculated in the analysis over the complete trajectory (red curve - last 100 ns), every one nanosecond in the last 100 ns (purple curve), every two nanoseconds in the last 100 ns (green curve), every 5 nanoseconds in the last 100 ns (blue curve), and every ten nanoseconds in the last 100 ns (yellow curve) were 7.40, 7.38, 7.25, 7.24 and 6.61 nm², respectively. These results indicate, for instance, that the analysis performed every five nanoseconds from the last 100 ns MD trajectory accesses a statistically relevant ensemble of structures generated in the MD simulation. The corresponding eigenvectors capture the essential protein motions in line with the results obtained considering the complete set of frames saved during the last 100 ns of simulation. We are highlighting the analysis performed every five nanoseconds because the structures used in the EPR parameters calculations were saved considering this time step along the final 100 ns of simulation.

To evaluate the correlation between the set of structures associated with the corresponding eigenvector of the covariance matrix built from the analysis with all snapshots saved in the MD trajectory and the ones saved every five nanoseconds, we plot the displacement vectors onto their first two principal PCs. The results are presented in Figure S4.

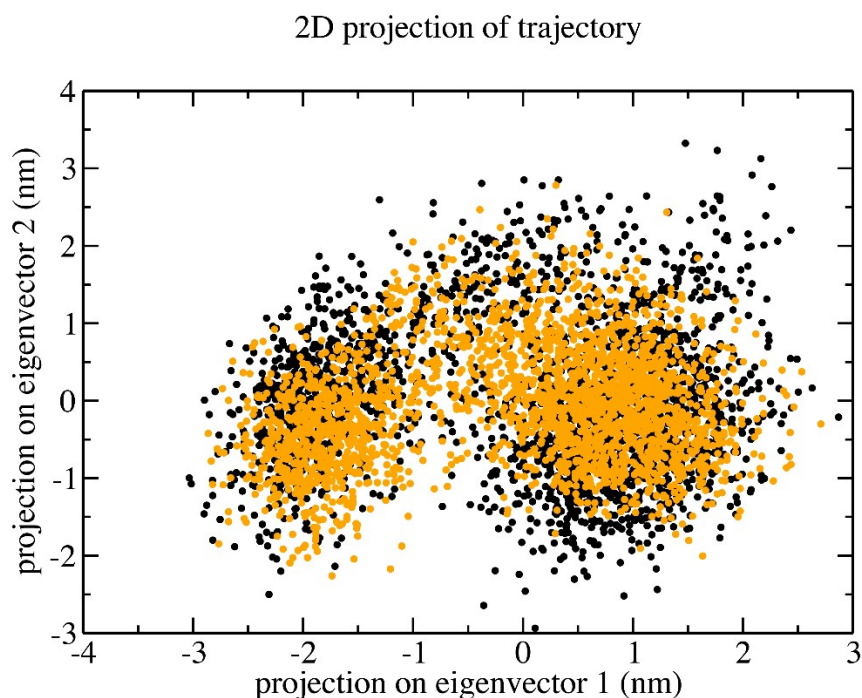


Figure S4: Projection of the protein backbone atoms in the phase space along the first two eigenvectors (PC 1 and PC2) obtained from the covariance matrix diagonalization built from the entire frames (black points) and from the analysis performed every five nanoseconds of the last 100 ns MD trajectory.

It is possible to see in Figure S4 that the MD trajectory accessed essential regions of the phase space with a non-uniform distribution that sampled, in this case, two crucial states of the protein according to the two clusters formed (denser region). Also, it's worth highlighting that the profile constructed from the analysis performed every five nanoseconds of the trajectory samples the essential phase space region yielded from the analysis carried out with the entire trajectory of the last 100 ns MD simulation.

To evaluate the convergence of the MD trajectory used in the PCA analysis, we calculated the cosine content (c.c.) of the first principal component of the covariance matrix. The results are quoted in Table S1.

Table S1: The first 20 principal components (PC_i), percentual cumulative normalized eigenvalues (CNE) (%) and the cosine content (C.C.) calculated for the respective modes of the condition 3 (frames saved every 5 nanoseconds).

PC(i)	Eigenvalue (i)	CNE (%)	C.C.
1	2.03	28.077	0.814645
2	1.05	14.523	0.046871
3	0.63	8.7137	0.162891
4	0.55	7.6072	0.000983
5	0.37	5.1176	0.008519
6	0.34	4.7026	0.012157
7	0.29	4.0111	0.008571
8	0.28	3.8728	0.000198
9	0.23	3.1812	0.008391
10	0.22	3.0429	0.046126
11	0.21	2.9046	0.050463
12	0.19	2.6279	0.001184
13	0.15	2.0747	0.003785
14	0.14	1.9364	0.025238
15	0.12	1.6598	0.001584
16	0.11	1.5214	0.000195
17	0.10	1.3831	0.001619
18	0.09	1.2448	0.008933
19	0.07	0.9682	0.003663
20	0.06	0.8299	0.003217

It has been reported that cosine content in the range of 0.2 to 0.5 produces a reliable minimum energy set of structures. Table S1 shows that the cosine content for the first mode is high, indicating that the associated eigenvector represents random motion in the system. All the other calculated cosine contents are close to zero, confirming the convergence of the simulation. It is worth highlighting that even if the first mode is removed, the sum of the modes two to ten captures more than 50 % of the protein motion. Furthermore, the MD trajectory was projected onto the 20 eigenvectors associated with the first eigenvalues of the covariance matrix. The results are presented in Figure S5.

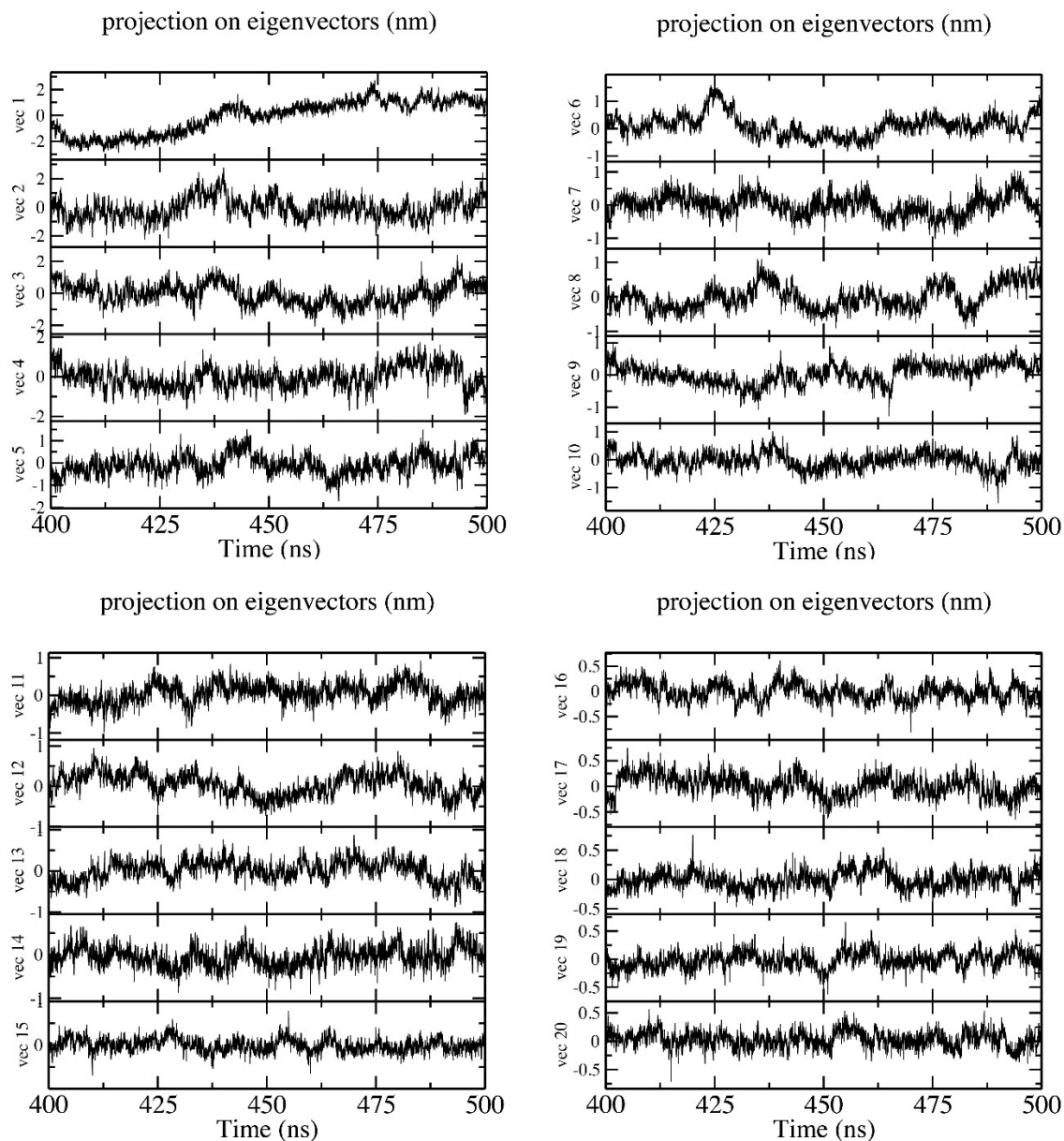


Figure S5: Projection of the MD trajectory over the 20 eigenvectors correspondent to the eigenvalues calculated from the covariance matrix diagonalization built from analysis performed on the last 100 ns MD simulation evaluated every five nanoseconds.

Overall, the analysis of Figure S5 indicates that the 20 eigenvectors corresponding to the first 20 eigenvalues obtained from the covariance matrix diagonalization in condition 3 (trajectory analyzed every five nanoseconds) describe different essential motions of the protein along the final 100 ns of the MD simulation. As can be seen, different profiles in the function of the time are observed for the first twenty modes.

The PCA analysis was carried out using `gmx_covar` and `gmx_anaeig` tools implemented in GROMACS code version 2018.3.⁶ Cosine content calculations for the first twenty PCs were performed using `gmx_analyse` tool.

5 - Integration grid effect on EPR parameters calculations

Besides the dependence concerning the XC functional, EPR parameters calculations also are sensitive to the basis set function and the integration grid.^{7,8} Thus, initially, we evaluated the effect of the integration grid on the computation of the g-factor and hyperfine coupling constant for the copper Cu_B site. As shown in Table S2, the results obtained considering an integral grid with 770 angular points per shell (Grid7) did not differ much from the one calculated with 434 points (Grid5), which in a way indicate the basis set used (def2-TZVP) is large enough to describe satisfactorily. At least in this case, where the atomic core region is essential to calculating the properties depending on the core spin-density. Furthermore, Hedegård and co-workers have shown in a very detailed systematic study concerning the calculations of EPR parameters of a lytic polysaccharide monooxygenase that def2-TZVP is indeed an adequate basis set function for the calculation of the depending on EPR spin-Hamiltonian properties.⁸ Therefore, all CPKS-DFT results were obtained from calculations performed using the def2-TZVP basis set and considering a sizeable integral grid with 434 angular points per shell.

Table S2: Calculated EPR parameters g and A^{Cu} (MHz) tensors, A_{iso} and contributions from the Fermi contact (A_{FC}) at the DFT/def2-TZVP level considering different integration grid (Grid5 and Grid7). Calculation carried out on the structure named as frame1 (see figure S5). CGTOs is the number of contracted Gaussian Type Orbitals functions in the basis set.

B1LYP									
Grid	CGTOs	$\mathbf{g_1}$	$\mathbf{g_2}$	$\mathbf{g_3}$	$\mathbf{A_{FC}}$	$\mathbf{A_{iso}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$\mathbf{A_3}$
Label ^a	2153	$\mathbf{g_y}$	$\mathbf{g_x}$	$\mathbf{g_z}$			$\mathbf{A_x}$	$\mathbf{A_y}$	$\mathbf{A_z}$
Grid5		2.050	2.088	2.207	110.5	269.12	-175.3	408.1	574.5
Grid7		2.050	2.088	2.207	110.9	269.52	-174.9	408.5	574.9
BHandHLYP									
Grid	CGTOs	$\mathbf{g_1}$	$\mathbf{g_2}$	$\mathbf{g_3}$	$\mathbf{A_{FC}}$	$\mathbf{A_{iso}}$	$\mathbf{A_1}$	$\mathbf{A_2}$	$\mathbf{A_3}$
Label ^a	2153	$\mathbf{g_y}$	$\mathbf{g_x}$	$\mathbf{g_z}$			$\mathbf{A_x}$	$\mathbf{A_y}$	$\mathbf{A_z}$
Grid5		2.068	2.122	2.301	103.8	323.5	-126.4	464.5	632.2
Grid7		2.069	2.122	2.301	104.4	324.0	-125.9	465.0	632.8

^a The labels were assigned according to the eigenvectors orientation concerning to the molecular reference model (frame1).

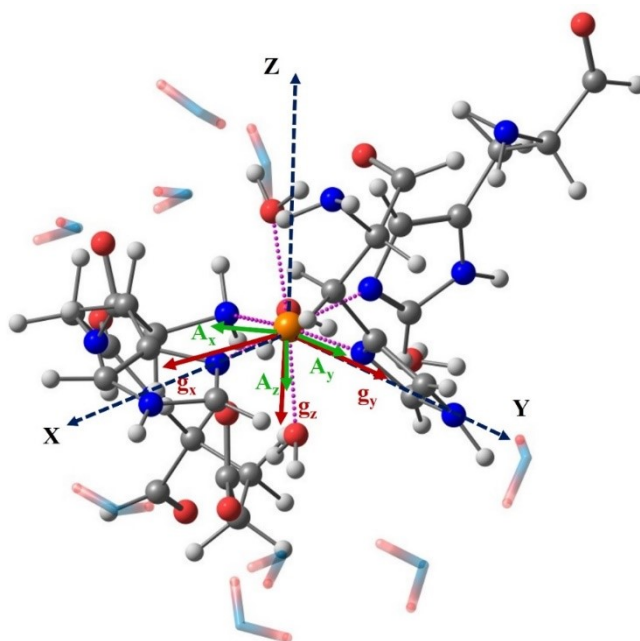


Figure S6: Structure of the frame1 cluster and the representation of the calculated relative orientation of the g -factor matrix (red) and A^{Cu} (green) tensor. The representation in the sticks corresponds to the water molecules within 5 Å from the copper ion generated from the MD simulation. The two water molecules directly bound to the copper are represented in ball stick format.

Table S3: Calculated EPR parameter g tensor with the hybrid GGA B1LYP and B3LYP functionals.

Frame	g^{B1LYP}_x	g^{B1LYP}_y	g^{B1LYP}_z	g^{B3LYP}_x	g^{B3LYP}_y	g^{B3LYP}_z
1	2.088	2.051	2.207	2.082	2.047	2.193
2	2.078	2.057	2.211	2.073	2.053	2.196
3	2.062	2.059	2.190	2.058	2.055	2.176
4	2.112	2.040	2.212	2.104	2.038	2.197
5	2.077	2.060	2.204	2.071	2.057	2.190
6	2.085	2.055	2.207	2.080	2.051	2.193
7	2.082	2.051	2.207	2.076	2.048	2.192
8	2.074	2.060	2.207	2.069	2.056	2.192
9	2.075	2.059	2.209	2.071	2.055	2.194
10	2.063	2.053	2.187	2.058	2.049	2.174
11	2.069	2.051	2.187	2.064	2.048	2.173
12	2.074	2.055	2.196	2.068	2.052	2.181
13	2.090	2.058	2.217	2.083	2.055	2.202
14	2.065	2.053	2.185	2.061	2.049	2.172
15	2.057	2.048	2.175	2.053	2.045	2.162
16	2.067	2.063	2.203	2.062	2.058	2.188
17	2.078	2.049	2.196	2.073	2.046	2.182
18	2.080	2.053	2.207	2.074	2.049	2.192
19	2.071	2.053	2.191	2.066	2.050	2.178
20	2.068	2.055	2.192	2.064	2.051	2.178
Average	2.076 ± 0.012	2.054 ± 0.005	2.199 ± 0.011	2.071 ± 0.011	2.051 ± 0.005	2.190 ± 0.012

Table S4: Calculated copper hyperfine constant with the hybrid GGA B1LYP and B3LYP functionals.

Frame	A^{B1LYP}_x	A^{B1LYP}_y	A^{B1LYP}_z	A^{B3LYP}_x	A^{B3LYP}_y	A^{B3LYP}_z
1	-175.3	408.1	574.5	-172.7	395.9	557.8
2	-197.6	424.7	499.0	-194.4	409.0	484.5
3	-229.5	424.2	453.3	-225.1	410.3	438.2
4	-139.8	387.2	620.8	-139.2	377.2	600.5
5	-209.1	436.5	494.1	-206.9	423.4	475.7
6	-184.8	419.6	548.5	-181.2	404.6	533.8
7	-179.7	419.6	552.0	-175.7	407.5	537.5
8	-209.2	417.1	492.6	-206.5	403.2	475.1
9	-208.5	432.5	494.4	-205.5	417.4	480.8
10	-240.8	399.8	462.4	-235.9	387.7	448.4
11	-213.6	419.8	510.0	-207.6	408.7	497.3
12	-214.5	407.0	500.3	-211.4	394.1	482.2
13	-178.3	432.9	548.6	-177.6	423.2	527.2
14	-238.3	407.1	466.7	-233.5	394.7	451.8
15	-242.5	390.4	455.5	-235.5	380.2	442.5
16	-227.1	434.2	460.7	-224.2	418.7	447.4
17	-206.5	404.6	522.4	-201.4	391.4	509.6
18	-192.9	406.0	516.8	-189.8	393.5	497.6
19	-223.4	411.4	489.0	-219.3	399.0	472.9
20	-232.7	410.5	467.1	-228.4	394.9	453.8
Average			506.0 ± 44.2			491.0 ± 43.0

6 - EPR parameters calculations for One-water Complexes

Table S5: g-factor and copper parallel hyperfine constant calculated with the hybrid GGA BHandLYP functional for one-water complex model 1.

Frame	$g^{BHandLYP}_x$	$g^{BHandLYP}_y$	$g^{BHandLYP}_z$	$A^{BHandLYP}_{\parallel}$
1	2.070	2.097	2.288	557.29
2	2.077	2.084	2.289	482.08
3	2.070	2.08	2.264	458.02
4	2.076	2.097	2.299	539.31
5	2.075	2.088	2.284	484.62
6	2.082	2.083	2.288	498.07
7	2.074	2.090	2.290	540.14
8	2.080	2.083	2.290	473.36
9	2.076	2.083	2.286	479.87
10	2.071	2.073	2.260	459.80
11	2.066	2.077	2.255	496.22
12	2.075	2.08	2.274	476.92
13	2.085	2.089	2.300	513.16
14	2.069	2.074	2.256	463.63
15	2.065	2.072	2.250	478.86
16	2.075	2.083	2.281	463.49
17	2.070	2.086	2.273	513.02
18	2.077	2.087	2.292	505.95
19	2.073	2.078	2.267	474.72
20	2.071	2.077	2.268	462.97
Average	2.074 ± 0.005	2.083 ± 0.01	2.278 ± 0.01	492.0 ± 28.0

Table S6: g-factor and copper parallel hyperfine constant calculated with the hybrid GGA BHandLYP functional for one-water complex model 2.

Frame	$g^{BHandLYP}_x$	$g^{BHandLYP}_y$	$g^{BHandLYP}_z$	$A^{BHandLYP}_{\parallel}$
1	2.074	2.093	2.289	540.23
2	2.075	2.090	2.293	497.97
3	2.072	2.077	2.265	474.57
4	2.07	2.107	2.299	574.39
5	2.073	2.091	2.283	506.71
6	2.07	2.098	2.286	543.36
7	2.066	2.093	2.286	540.49
8	2.082	2.091	2.295	514.94
9	2.079	2.086	2.291	492.8
10	2.064	2.081	2.26	494.42

11	2.067	2.086	2.262	533.64
12	2.071	2.088	2.276	510.63
13	2.078	2.101	2.301	542.71
14	2.069	2.074	2.256	542.48
15	2.060	2.070	2.243	462.54
16	2.075	2.082	2.280	472.72
17	2.068	2.085	2.271	503.11
18	2.071	2.094	2.29	524.67
19	2.071	2.081	2.673	485.05
20	2.075	2.079	2.271	472.47
Average	2.072 ± 0.005	2.090 ± 0.01	2.229 ± 0.01	512.0 ± 30.0

Table S7: Hyperfine coupling constants calculated for the water's protons in the pentacoordinate complex model 1.

Frame	$A_{\parallel}^{Ha}$	$A_{\parallel}^{Hb}$	$A_{\perp}^{Ha}$	$A_{\perp}^{Hb}$
1	1.63	1.92	-0.85	-0.91
2	4.9	5.96	-2.63	-2.86
3	5.31	6.06	-2.81	-3.04
4	7.27	6.70	-3.48	-3.39
5	6.34	5.51	-3.15	-2.87
6	6.06	5.97	-3.13	-3.07
7	5.28	7.08	-2.97	-3.52
8	5.83	5.18	-2.75	-2.48
9	6.36	5.52	-3.16	-2.77
10	4.42	5.44	-2.50	-2.61
11	3.80	6.07	-2.26	-2.81
12	5.20	6.06	-2.75	-2.97
13	4.97	6.76	-2.83	-3.19
14	6.22	5.73	-3.22	-2.95
15	5.79	5.56	-2.95	-2.89
16	5.03	6.61	-2.94	-3.19
17	5.35	7.24	-2.94	-3.54
18	4.74	7.28	-2.77	-3.47
19	5.44	5.82	-2.86	-2.97
20	5.14	6.61	-2.45	-2.46
Average	5.25 ± 1.12	5.95 ± 1.11	-2.77 ± 0.52	-2.90 ± 0.55

Table S8: Hyperfine coupling constants calculated for the water's protons in the pentacoordinate complex model 2.

Frame	$A_{\parallel}^{Hc}$	$A_{\parallel}^{Hd}$	$A_{\perp}^{Hc}$	$A_{\perp}^{Hd}$
1	1.38	1.63	-0.75	-0.78
2	6.21	6.49	-3.265	-3.41

3	6.68	5.51	-3.245	-2.89
4	6.65	7.14	-3.75	-3.66
5	5.31	8.12	-2.98	-4.02
6	6.19	7.83	-3.29	-3.84
7	5.44	5.68	-2.59	-2.74
8	5.56	7.13	-3.10	-3.60
9	5.93	6.63	-3.13	-3.34
10	5.59	6.43	-2.71	-3.16
11	5.57	6.24	-2.96	-3.11
12	5.93	8.38	-3.21	-4.04
13	1.50	1.62	-0.73	-0.77
14	5.46	5.31	-2.84	-2.78
15	5.28	3.60	-2.48	-2.02
16	5.68	5.04	-2.89	-2.66
17	5.82	5.06	-2.84	-2.68
18	6.43	4.89	-3.04	-2.50
19	4.52	6.94	-2.62	-3.32
20	7.79	5.17	-3.74	-2.96
<i>Average</i>	5.63 ± 1.12	5.93 ± 1.11	-2.90 ± 0.62	-3.00 ± 0.76

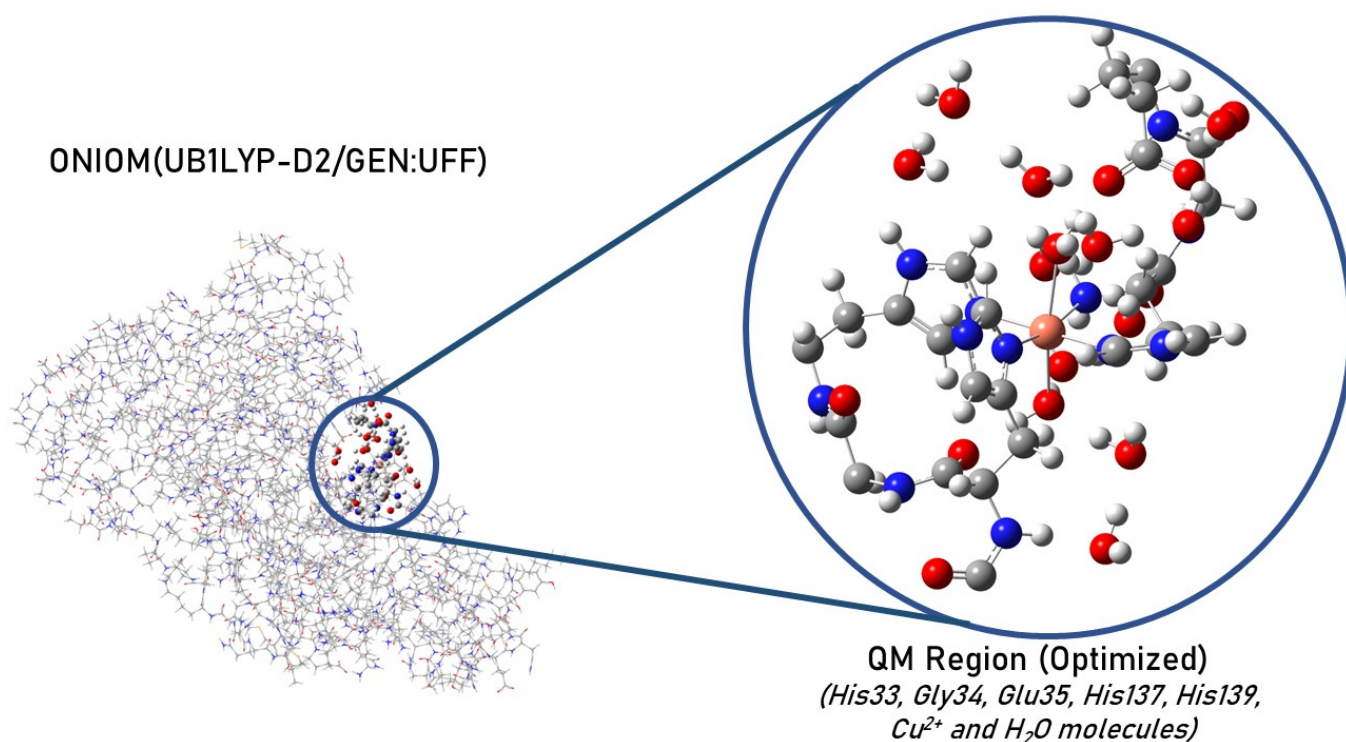


Figure S7: ONIOM QM/MM optimized structure with highlights to the QM region.

Figure S8 shows the spin density calculated on MD and QM/MM structures. As can be seen the profiles are quite similar, indicating that the Cu_B site has a significant spin on copper ion,

as expected, given of the Cu(II) oxidation state. Furthermore, the calculated spin density analysis also suggests that the unpaired electron of Cu(II) ion is located essentially in a $d_{x^2-y^2}$ orbital. The spin density is also spread over the nitrogenous ligands of the His³³, His¹³⁷, and His¹³⁹ residues directly bound to copper ion.

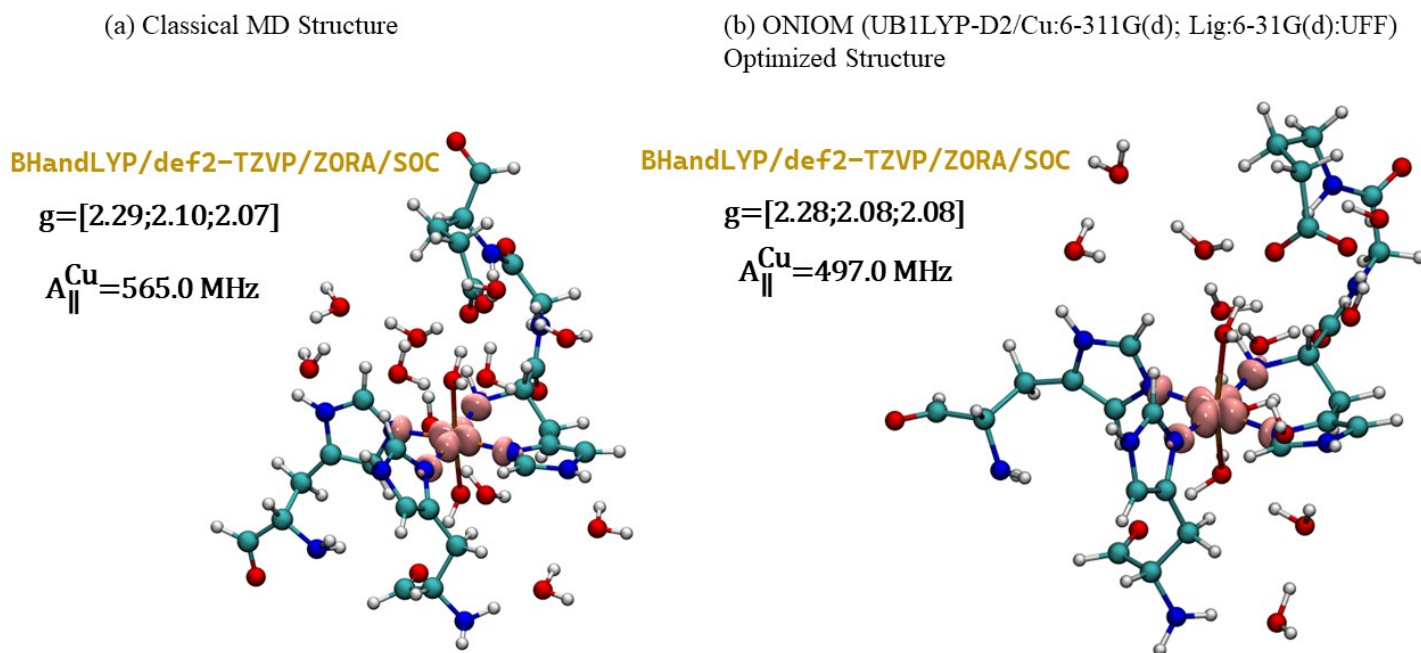


Figure S8: Spin-density (iso value of 0.07) and EPR parameters calculated at the BHANDLYP/def2-TZVP level over (a) a structure came from a MD simulation and (b) over the QM region of an optimized QM/MM geometry.

7 – Cartesian coordinates of the 20 frames used in the EPR calculations

Di-aqua Complexes

Frame 1:				Frame 2:			
N	0.28396000	-1.38673000	0.05140000	N	0.81730000	-0.58622000	-0.27784000
H	-0.28604000	-1.57673000	-0.75860000	H	0.42730000	-0.76622000	-1.19784000
H	-0.13604000	-1.96673000	0.77140000	H	0.97730000	-1.56622000	-0.05784000
C	1.37396000	-2.25673000	-0.33860000	C	2.17730000	-0.25622000	-0.65784000
H	1.66396000	-1.92673000	-1.33860000	H	2.16730000	0.46378000	-1.47784000
C	2.48396000	-2.05673000	0.69140000	C	3.06730000	0.26378000	0.46216000
H	2.19396000	-2.10673000	1.74140000	H	2.95730000	-0.18622000	1.44216000
H	3.22396000	-2.83673000	0.55140000	H	4.11730000	0.15378000	0.19216000
C	3.23396000	-0.77673000	0.43140000	C	2.75730000	1.73378000	0.59216000
N	2.62396000	0.47327000	0.32140000	N	1.56730000	2.10378000	1.21216000
C	4.58396000	-0.66673000	0.23140000	C	3.50730000	2.78378000	0.13216000
H	5.42396000	-1.34673000	0.26140000	H	4.47730000	2.79379000	-0.34784000
C	3.61396000	1.34327000	0.13140000	C	1.69729000	3.43378000	1.22216000
H	3.45396000	2.39327000	-0.02860000	H	0.97730000	4.15378000	1.58216000
N	4.79396000	0.70327000	0.19140000	N	2.80730000	3.87378000	0.61216000
H	5.67396000	1.15327000	-0.00860000	H	3.01729000	4.86378000	0.53216000
C	0.90396000	-3.70673000	-0.31860000	C	2.76729000	-1.52621000	-1.24784000
O	0.75396000	-4.23673000	0.77140000	O	2.59730000	-2.56622000	-0.61784000
N	0.64396000	-4.42673000	-1.40860000	N	3.24730000	-1.45621000	-2.48784000
H	0.74396000	-3.94673000	-2.28860000	H	3.50730000	-0.53622000	-2.79784000
C	-0.07604000	-5.68673000	-1.42860000	C	3.71730000	-2.61621000	-3.22784000
H	0.65396000	-6.45673000	-1.66860000	H	4.69729000	-2.44622000	-3.67784000
H	-0.51604000	-5.92673000	-0.45860000	H	3.97730000	-3.43622000	-2.54784000
C	-1.17604000	-5.70673000	-2.47860000	C	2.87729000	-3.09622000	-4.38784000
O	-1.97604000	-6.63673000	-2.43860000	O	3.34730000	-3.87622000	-5.21784000
N	-1.32604000	-4.63673000	-3.26860000	N	1.61730000	-2.65622000	-4.47784000
H	-0.77604000	-3.82673000	-3.01860000	H	1.30730000	-2.09622000	-3.70784000
C	-2.25604000	-4.38673000	-4.34860000	C	0.74730000	-2.68622000	-5.63784000
H	-3.24604000	-4.60673000	-3.94860000	H	0.63730000	-3.72622000	-5.95784000
C	-2.27604000	-2.88673000	-4.62860000	C	-0.67270000	-2.25622000	-5.25784000
H	-3.02604000	-2.61673000	-5.36860000	H	-1.29270000	-2.52621000	-6.11784000
H	-2.70604000	-2.36673000	-3.77860000	H	-1.01270000	-2.89622000	-4.43784000
C	-1.01604000	-2.04673000	-4.87860000	C	-0.84270000	-0.77621000	-4.93784000
H	-0.30604000	-2.51673000	-5.55860000	H	-0.39270000	-0.11621000	-5.67784000
H	-1.30604000	-1.10673000	-5.34860000	H	-1.90270000	-0.52621000	-5.02784000
C	-0.20604000	-1.64673000	-3.65860000	C	-0.33270000	-0.30622000	-3.57784000
O	-0.54604000	-2.02673000	-2.51860000	O	-0.41270000	-1.13622000	-2.64784000
O	0.69396000	-0.78673000	-3.76860000	O	0.37730000	0.72379000	-3.52784000
C	-2.10604000	-5.11673000	-5.66860000	C	1.27730000	-2.07622000	-6.92784000
O	-3.09550351	-5.23781443	-6.43663065	O	0.62521528	-2.20038789	-7.99692298
N	2.92396000	3.54327000	4.86140000	N	-0.43270000	2.32378000	6.69216000
H	3.61172000	2.93662000	4.46270000	H	0.45936390	2.01654772	6.36075341
C	1.91396000	3.84327000	3.87140000	C	-1.36270000	2.39378000	5.58216000
H	1.93396000	4.90327000	3.63140000	H	-2.00270000	3.26378000	5.69216000
C	2.29396000	3.10327000	2.59140000	C	-0.62270000	2.30378000	4.24216000
H	3.33396000	3.37327000	2.39140000	H	0.31730000	2.86378000	4.31216000
H	2.18396000	2.02327000	2.65140000	H	-0.26270000	1.28378000	4.08216000
C	1.44396000	3.46327000	1.40140000	C	-1.19270000	2.93378000	3.00216000
N	0.73396000	2.55327000	0.63140000	N	-1.11270000	2.39378000	1.72216000
C	1.35396000	4.70327000	0.83140000	C	-2.02270000	4.02378000	2.99216000
H	1.74396000	5.64327000	1.19140000	H	-2.40270000	4.62378000	3.80216000
C	0.08396000	3.31327000	-0.24860000	C	-1.71270000	3.26378000	0.91216000
H	-0.50604000	3.05327000	-1.10860000	H	-1.80270000	3.20378000	-0.15784000
N	0.36396000	4.62327000	-0.12860000	N	-2.26270000	4.24378000	1.65216000
H	0.16396000	5.29327000	-0.86860000	H	-2.85270000	5.00378000	1.34216000

C	0.62396000	3.33327000	4.51140000	C	-2.11270000	1.07378000	5.72216000
O	0.38957000	2.09771000	4.55626000	O	-1.47577202	-0.01088251	5.75958402
N	-2.83604000	2.90327000	4.32140000	N	-5.03270000	-0.99622000	3.88216000
H	-2.55784000	1.97985000	4.58577000	H	-5.00520835	-1.84918367	4.40340580
C	-4.14604000	2.85327000	3.69140000	C	-5.73270000	-1.21622000	2.63216000
H	-4.24604000	3.56327000	2.87140000	H	-6.07270000	-0.27621000	2.19216000
C	-4.30604000	1.48327000	3.04140000	C	-4.77270000	-2.00622000	1.73216000
H	-4.01604000	0.69327000	3.73140000	H	-4.35270000	-2.85622000	2.26216000
H	-5.32604000	1.21327000	2.77140000	H	-5.37270000	-2.41622000	0.92216000
C	-3.39604000	1.29327000	1.86140000	C	-3.65270000	-1.26622000	1.06216000
N	-3.72604000	1.16327000	0.52140000	N	-3.68270000	-0.93622000	-0.27784000
H	-4.65604000	1.28327000	0.15140000	H	-4.41270000	-1.18622000	-0.93784000
C	-2.08604000	0.92327000	1.96140000	C	-2.41270000	-0.87622000	1.50216000
H	-1.52604000	0.81327000	2.88140000	H	-1.94270000	-1.02621000	2.46216000
C	-2.59604000	0.79327000	-0.09860000	C	-2.59270000	-0.19622000	-0.51784000
H	-2.62604000	0.67327000	-1.16860000	H	-2.28270000	0.19378000	-1.47784000
N	-1.52604000	0.70327000	0.70140000	N	-1.77270000	-0.11621000	0.52216000
C	-5.24604000	3.02327000	4.72140000	C	-6.88270000	-2.17622000	2.92216000
O	-4.98647000	2.89550000	5.94609000	O	-6.67788279	-3.21720891	3.59888931
O	2.69396000	2.38327000	-3.10860000	Cu	-0.04270000	0.90378000	0.74216000
H	2.53396000	1.90327000	-3.91860000	O	4.07730000	2.31378000	4.41216000
H	3.64396000	2.45327000	-3.04860000	H	4.60730000	2.69378000	3.72216000
O	3.39396000	-1.29673000	-3.13860000	H	4.47730000	2.63379000	5.22216000
H	2.45396000	-1.29673000	-3.33860000	O	2.31730000	-4.10622000	1.60216000
H	3.58396000	-2.19673000	-2.88860000	H	3.06730000	-4.67622000	1.74216000
O	0.03396000	-2.49673000	3.89140000	H	2.38730000	-3.83622000	0.68216000
H	-0.75604000	-2.62673000	3.36140000	O	-4.17270000	2.49378000	-1.41784000
H	0.21396000	-3.35673000	4.26140000	H	-3.72270000	3.21378000	-1.86784000
O	-2.07604000	-2.58673000	2.13140000	H	-4.17270000	1.77378000	-2.05784000
H	-2.49604000	-3.36673000	2.50140000	O	3.69729000	-1.66622000	3.35216000
H	-2.24604000	-2.64673000	1.19140000	H	3.51729000	-2.49622000	2.90216000
O	-2.48604000	-2.22673000	-0.99860000	H	4.54730000	-1.39622000	3.01216000
H	-1.74604000	-2.13673000	-1.59860000	O	2.09730000	2.72379000	-4.06784000
H	-3.22604000	-1.83673000	-1.46860000	H	1.41730000	2.05378000	-4.01784000
O	4.70396000	-1.41673000	3.21140000	H	2.08729000	3.00378000	-4.98784000
H	5.64396000	-1.60673000	3.18140000	O	0.87729000	4.53378000	-2.10784000
H	4.28396000	-2.23673000	2.94140000	H	1.49730000	4.14378000	-2.71784000
O	0.59396000	0.78327000	-1.71860000	H	0.12730000	4.79379000	-2.64784000
H	1.25396000	1.38327000	-2.05860000	O	-0.26270000	-2.78622000	1.35216000
H	0.46396000	0.14327000	-2.40860000	H	0.39730000	-3.41622000	1.64216000
O	-2.89604000	3.69327000	-2.33860000	H	-0.72270000	-3.22622000	0.64216000
H	-2.41604000	3.65327000	-3.16860000	O	-0.08270000	2.15378000	-1.25784000
H	-3.51604000	2.96327000	-2.37860000	H	0.19730000	3.03378000	-1.49784000
O	0.50396000	-0.11673000	2.70140000	H	-0.10270000	1.67378000	-2.08784000
H	0.50396000	0.57327000	3.37140000	O	-3.23270000	-1.74622000	-3.12784000
H	0.16396000	-0.88673000	3.15140000	H	-3.54270000	-2.24622000	-3.88784000
O	2.01396000	0.77327000	-5.32860000	H	-2.28270000	-1.87622000	-3.13784000
H	1.35396000	1.41327000	-5.58860000	O	0.50730000	-0.26622000	2.49216000
H	1.55396000	0.18327000	-4.72860000	H	1.14730000	-0.04622000	3.17216000
O	4.18396000	0.92327000	4.52140000	H	0.38730000	-1.21622000	2.56216000
H	4.03396000	0.02327000	4.24140000	O	2.04730000	0.16378000	4.83216000
H	5.13396000	1.01327000	4.53140000	H	2.65730000	0.86378000	4.59216000
O	-4.42604000	-0.71673000	-2.15860000	H	2.53730000	-0.64622000	4.65216000
H	-4.73604000	0.19327000	-2.09860000	O	-0.40270000	-3.58622000	-1.24784000
H	-5.21604000	-1.21673000	-2.37860000	H	-0.08270000	-4.13622000	-1.96784000
O	0.56396000	4.17327000	-3.39860000	H	-0.44270000	-2.70621000	-1.62784000
H	1.15396000	3.55327000	-2.95860000	H	-5.51053342	-0.29637351	4.41309325
H	0.66396000	3.97327000	-4.32860000	H	-7.86329213	-1.96428280	2.55010934
Cu	0.57396000	0.48327000	0.46140000	H	2.20431087	-1.54185515	-6.92559189
H	-0.08026000	4.02664000	4.92152000	H	-3.18062782	1.06966540	5.78859215
H	3.36078000	4.39192000	5.15970000	H	-0.34042808	3.22884583	7.10730062
H	-2.17054000	3.28031000	3.67723000				
H	-6.24287000	3.25186000	4.40680000				
H	-1.15883174	-5.52906219	-5.94730894				
Frame 3:				Frame 4:			
N	0.90711000	-0.10588000	-0.23930000	N	1.05088000	-0.27588000	-0.08386000
H	0.72711000	-0.38588000	-1.18930000	H	0.92088000	-0.97588000	-0.79386000

H	1.20710000	-0.90588000	0.30070000	H	1.00088000	-0.90588000	0.70614000
C	2.23711000	0.44412000	-0.35930000	C	2.49088000	-0.09588000	-0.14386000
H	2.40711000	1.19412000	-1.13930000	H	2.84088000	0.05412000	-1.16386000
C	2.76711000	1.13412000	0.90070000	C	3.01088000	1.10412000	0.63614000
H	2.67710000	0.39412000	1.70070000	H	2.67088000	1.17412000	1.66614000
H	3.84711000	1.29412000	0.87070000	H	4.10088000	1.09412000	0.68614000
C	2.09711000	2.46412000	1.15070000	C	2.63088000	2.42412000	0.01614000
N	0.71710000	2.50412000	1.02070000	N	1.32088000	2.67412000	-0.37386000
C	2.54711000	3.75412000	1.19070000	C	3.42088000	3.48412000	-0.35386000
H	3.57710000	4.07412000	1.19070000	H	4.48088000	3.66412000	-0.24386000
C	0.41711000	3.79412000	1.11070000	C	1.40088000	3.82412000	-1.04386000
H	-0.60290000	4.12412000	0.98070000	H	0.61088000	4.26412000	-1.63386000
N	1.47711000	4.62412000	1.13070000	N	2.65088000	4.30412000	-1.14386000
H	1.43711000	5.63412000	1.01070000	H	2.97088000	5.17412000	-1.55386000
C	3.10710000	-0.77588000	-0.59930000	C	3.11088000	-1.41588000	0.29614000
O	3.00711000	-1.73588000	0.15070000	O	2.86088000	-1.83588000	1.42614000
N	3.67710000	-0.84588000	-1.80930000	N	3.91088000	-2.08588000	-0.53386000
H	3.58711000	-0.11588000	-2.48930000	H	4.18088000	-1.69588000	-1.42386000
C	4.48711000	-1.94588000	-2.29930000	C	4.24088000	-3.47588000	-0.27386000
H	5.51711000	-1.59588000	-2.33930000	H	5.32088000	-3.49588000	-0.16386000
H	4.52710000	-2.68588000	-1.49930000	H	3.91088000	-3.91588000	0.66614000
C	3.86711000	-2.60588000	-3.52930000	C	3.71088000	-4.35588000	-1.39386000
O	3.84711000	-3.83588000	-3.55930000	O	3.28088000	-5.49588000	-1.21386000
N	3.41711000	-1.76588000	-4.45930000	N	3.69088000	-3.80588000	-2.61386000
H	3.41711000	-0.77588000	-4.29930000	H	3.99088000	-2.84588000	-2.60386000
C	2.63710000	-2.11588000	-5.63930000	C	3.24088000	-4.43588000	-3.84386000
H	3.06710000	-3.07588000	-5.91930000	H	3.52088000	-5.49588000	-3.82386000
C	1.14710000	-2.31588000	-5.33930000	C	1.72088000	-4.33588000	-3.94386000
H	0.76711000	-2.93588000	-6.13930000	H	1.44088000	-4.96588000	-4.78386000
H	0.99710000	-3.10588000	-4.59930000	H	1.19088000	-4.74588000	-3.08386000
C	0.21710000	-1.19588000	-4.86930000	C	1.18088000	-2.91588000	-4.15386000
H	0.35710000	-0.28588000	-5.44930000	H	1.72088000	-2.44588000	-4.97386000
H	-0.84289000	-1.36588000	-5.01930000	H	0.19088000	-2.98588000	-4.61386000
C	0.28710000	-0.76588000	-3.41930000	C	1.08088000	-2.02588000	-2.92386000
O	0.07710000	-1.64588000	-2.55930000	O	0.54088000	-2.47588000	-1.89386000
O	0.61711000	0.41412000	-3.14930000	O	1.60088000	-0.89588000	-3.02386000
C	2.94711000	-1.22588000	-6.83930000	C	3.93088000	-4.16588000	-5.16386000
O	2.23628082	-1.29642495	-7.87530958	O	3.39296622	-4.53107352	-6.24128889
N	-0.92290000	1.67412000	6.72070000	N	-2.48912000	5.13412000	4.05614000
H	-0.16440771	1.02612279	6.65149692	H	-1.49021103	5.17984758	4.04666029
C	-1.67290000	1.67412000	5.48070000	C	-2.95912000	4.53412000	2.81614000
H	-2.53290000	2.33412000	5.48070000	H	-3.60912000	5.28412000	2.37614000
C	-0.88289000	2.13412000	4.25070000	C	-1.72912000	4.32412000	1.92614000
H	-0.34289000	3.02412000	4.58070000	H	-1.23912000	5.30412000	1.93614000
H	-0.07289000	1.42412000	4.08070000	H	-0.85912000	3.75412000	2.25614000
C	-1.73289000	2.40412000	3.05070000	C	-1.95912000	3.92412000	0.49614000
N	-1.96290000	1.50412000	2.01070000	N	-1.64912000	2.69412000	-0.07386000
C	-2.59289000	3.46412000	2.91070000	C	-2.46912000	4.71412000	-0.49386000
H	-2.89290000	4.29412000	3.54070000	H	-2.90912000	5.70412000	-0.50386000
C	-2.97289000	1.99412000	1.27070000	C	-2.16912000	2.69412000	-1.30386000
H	-3.31289000	1.72412000	0.29070000	H	-2.27912000	1.78412000	-1.87386000
N	-3.25289000	3.23412000	1.72070000	N	-2.54912000	3.94412000	-1.63386000
H	-3.78290000	3.94412000	1.23070000	H	-2.86912000	4.27412000	-2.52386000
C	-2.15289000	0.25412000	5.22070000	C	-3.63912000	3.23412000	3.20614000
O	-1.35346744	-0.60808435	4.77226071	O	-2.95477645	2.19117589	3.37200757
N	-4.76290000	-2.35588000	3.63070000	N	-5.54912000	0.31412000	2.71614000
H	-3.83983256	-2.72791508	3.72835450	H	-5.16815393	0.02318340	3.59376221
C	-5.30290000	-2.73588000	2.34070000	C	-5.84912000	-0.85588000	1.90614000
H	-5.85290000	-1.92588000	1.87070000	H	-6.24912000	-0.44588000	0.97614000
C	-4.21290000	-3.23588000	1.39070000	C	-4.63912000	-1.79588000	1.95614000
H	-3.57289000	-3.97588000	1.87070000	H	-4.26912000	-1.95588000	2.96614000
H	-4.68289000	-3.87588000	0.65070000	H	-4.86912000	-2.82588000	1.67614000
C	-3.31289000	-2.18588000	0.79070000	C	-3.49912000	-1.27588000	1.12614000
N	-3.29289000	-1.93588000	-0.56930000	N	-3.31912000	-1.68588000	-0.17386000
H	-3.91289000	-2.23588000	-1.29930000	H	-3.87912000	-2.35588000	-0.69386000
C	-2.23289000	-1.55588000	1.34070000	C	-2.53912000	-0.32588000	1.35614000
H	-1.98289000	-1.67588000	2.39070000	H	-2.37912000	0.27412000	2.24614000

C	-2.43289000	-0.91588000	-0.71930000	C	-2.29912000	-0.95588000	-0.66386000
H	-2.16289000	-0.50588000	-1.68930000	H	-2.03912000	-1.04588000	-1.70386000
N	-1.67290000	-0.72588000	0.37070000	N	-1.73912000	-0.14588000	0.23614000
C	-6.29289000	-3.87588000	2.52070000	C	-7.03912000	-1.55588000	2.53614000
O	-6.02694973	-4.82196071	3.30668831	O	-7.04192707	-1.80504706	3.76962225
Cu	-0.48289000	0.83412000	0.76070000	Cu	-0.16912000	1.28412000	-0.04386000
O	1.30711000	-2.74588000	3.31070000	O	-0.66912000	1.71412000	5.69614000
H	1.96710000	-3.27588000	2.86070000	H	-1.47912000	1.44412000	5.24614000
H	0.46710000	-3.10588000	3.02070000	H	-0.01912000	1.08412000	5.39614000
O	1.27710000	2.85412000	-2.96930000	O	-1.76912000	-0.81588000	4.59614000
H	1.00711000	1.95412000	-3.13930000	H	-1.65912000	-1.55588000	3.99614000
H	1.59711000	3.17412000	-3.80930000	H	-2.55912000	-1.02588000	5.09614000
O	3.53710000	1.01412000	-3.79930000	O	-3.50912000	0.82412000	-3.52386000
H	2.63710000	1.30412000	-3.61930000	H	-3.27912000	1.29412000	-4.32386000
H	4.07710000	1.72412000	-3.44930000	H	-3.28912000	-0.08588000	-3.70386000
O	-0.05290000	-4.37588000	1.61070000	O	2.09088000	0.27412000	4.73614000
H	0.22711000	-4.28588000	0.70070000	H	2.26088000	1.16412000	4.41614000
H	0.33711000	-5.19588000	1.90070000	H	2.78088000	-0.25588000	4.33614000
O	1.16711000	-3.78588000	-0.81930000	O	0.89088000	2.81412000	-3.91386000
H	1.99710000	-3.37588000	-0.57930000	H	0.72088000	2.33412000	-4.72386000
H	0.72711000	-3.12588000	-1.34930000	H	0.59088000	3.70412000	-4.09386000
O	-4.84289000	1.34412000	-2.33930000	O	-1.27912000	-2.89588000	2.97614000
H	-4.27289000	2.10412000	-2.45930000	H	-0.87912000	-3.65588000	3.39614000
H	-4.38289000	0.62412000	-2.76930000	H	-1.05912000	-2.98588000	2.04614000
O	1.71710000	0.68412000	6.70070000	O	-2.72912000	-1.85588000	-3.93386000
H	2.16711000	1.34412000	7.23070000	H	-2.96912000	-1.82588000	-4.85386000
H	2.27710000	0.55412000	5.94070000	H	-2.59912000	-2.78588000	-3.74386000
O	3.35710000	0.05412000	4.65070000	O	3.54088000	0.42412000	-4.61386000
H	4.20710000	-0.35588000	4.81070000	H	3.51088000	0.34412000	-5.56386000
H	2.75711000	-0.67588000	4.51070000	H	2.74088000	-0.00588000	-4.30386000
O	-0.91289000	1.61412000	-1.40930000	O	-0.11912000	0.82412000	-2.23386000
H	-0.34289000	1.27412000	-2.09930000	H	0.51088000	0.17412000	-2.54386000
H	-1.06289000	2.52412000	-1.64930000	H	0.06088000	1.60412000	-2.76386000
O	-0.84289000	4.32412000	-2.00930000	O	3.96088000	-1.16588000	3.71614000
H	-0.02289000	4.00412000	-2.36930000	H	3.54088000	-1.56588000	2.96614000
H	-1.48289000	4.20412000	-2.70930000	H	4.28088000	-1.90588000	4.23614000
O	-1.77289000	-3.39588000	-3.09930000	O	1.87088000	2.73412000	3.46614000
H	-1.14290000	-4.09588000	-3.28930000	H	2.54088000	3.40412000	3.37614000
H	-1.22289000	-2.62588000	-2.95930000	H	1.23088000	3.10412000	4.07614000
O	-0.97289000	7.00412000	-1.51930000	O	-0.11912000	1.43412000	2.03614000
H	-1.01290000	6.05412000	-1.56930000	H	-0.67912000	1.00412000	2.68614000
H	-1.68289000	7.30412000	-2.07930000	H	0.60088000	1.79412000	2.54614000
O	0.22711000	-0.40588000	2.48070000	O	-0.07912000	-3.33588000	0.54614000
H	0.75711000	-1.19588000	2.55070000	H	0.16088000	-3.21588000	-0.37386000
H	-0.33289000	-0.42588000	3.26070000	H	0.46088000	-4.06588000	0.84614000
H	-7.21566290	-3.87364910	1.97904956	H	-7.87577532	-1.83757091	1.93152599
H	-4.72914092	-1.35867016	3.69727965	H	-6.38825481	0.83486930	2.87321623
H	-1.52355926	1.40504072	7.47356439	H	-2.86424071	6.05701505	4.14302599
H	-3.17022416	-0.01150280	5.41913322	H	-4.70030438	3.20461856	3.33999580
H	3.76891276	-0.54178385	-6.79989583	H	4.87599391	-3.66450887	-5.18079223
Frame 5:				Frame 6:			
N	0.83820000	-0.46459000	-0.09261000	N	1.06667000	0.21991000	-0.16623000
H	0.45820000	-1.33459000	-0.42261000	H	0.86667000	-0.75009000	-0.36623000
H	1.09820000	-0.77460000	0.82739000	H	1.71667000	0.09991000	0.60377000
C	2.04820000	-0.61460000	-0.87261000	C	2.06667000	0.51991000	-1.16623000
H	1.53820000	-0.95460000	-1.77261000	H	1.78667000	0.12991000	-2.14623000
C	2.74819000	0.74540000	-0.94261000	C	2.18666000	2.03991000	-1.29623000
H	2.91820000	1.00541000	0.10739000	H	2.25667000	2.44991000	-0.28623000
H	3.68820000	0.61541000	-1.47261000	H	3.08667000	2.24991000	-1.86623000
C	1.98820000	1.79540000	-1.69261000	C	0.95667000	2.65991000	-1.90623000
N	0.73820000	2.27541000	-1.31261000	N	-0.32333000	2.51991000	-1.39623000
C	2.34820000	2.43541000	-2.85261000	C	0.94667000	3.41991000	-3.04623000
H	3.23820000	2.24540000	-3.42261000	H	1.72667000	3.67991000	-3.75623000
C	0.39820000	3.16541000	-2.23261000	C	-1.07333000	3.06991000	-2.35623000
H	-0.48180000	3.79540000	-2.23261000	H	-2.14333000	3.19991000	-2.27623000
N	1.27820000	3.20541000	-3.25261000	N	-0.38333000	3.58991000	-3.38623000
H	1.15820000	3.83540000	-4.03261000	H	-0.79333000	4.02991000	-4.19623000

C	2.95820000	-1.75460000	-0.43261000	C	3.38667000	-0.11009000	-0.73623000
O	3.17820000	-1.84460000	0.77739000	O	3.93666000	0.11991000	0.33377000
N	3.60820000	-2.40459000	-1.39261000	N	3.91667000	-1.00009000	-1.58623000
H	3.38820000	-2.21459000	-2.36261000	H	3.48667000	-1.13009000	-2.48623000
C	4.40820000	-3.60459000	-1.26261000	C	4.99667000	-1.94009000	-1.33623000
H	5.27820000	-3.42459000	-1.88261000	H	5.78667000	-1.63009000	-2.01623000
H	4.57820000	-3.80459000	-0.20261000	H	5.45667000	-1.84009000	-0.35623000
C	3.67820000	-4.87459000	-1.68261000	C	4.74667000	-3.43009000	-1.54623000
O	4.33820000	-5.90459000	-1.62261000	O	5.68667000	-4.19009000	-1.77623000
N	2.34820000	-4.82460000	-1.82261000	N	3.47667000	-3.81009000	-1.42623000
H	1.81820000	-3.96459000	-1.89261000	H	2.69667000	-3.20009000	-1.24623000
C	1.52820000	-5.99459000	-2.04261000	C	2.90667000	-5.07009000	-1.85623000
H	1.88820000	-6.88459000	-1.52261000	H	3.38667000	-5.83009000	-1.24623000
C	0.03820000	-5.77460000	-1.78261000	C	1.39667000	-5.16009000	-1.63623000
H	-0.57180000	-6.63459000	-2.07261000	H	1.02666000	-6.18009000	-1.72623000
H	-0.12180000	-5.56459000	-0.72261000	H	1.14667000	-4.93009000	-0.60623000
C	-0.57180000	-4.60459000	-2.56261000	C	0.51667000	-4.22009000	-2.47623000
H	-0.27180000	-4.74459000	-3.60261000	H	0.79667000	-4.25009000	-3.52623000
H	-1.65180000	-4.54459000	-2.54261000	H	-0.50333000	-4.58009000	-2.31623000
C	-0.22180000	-3.18460000	-2.15261000	C	0.50667000	-2.76009000	-2.05623000
O	-0.09180000	-2.29459000	-3.01261000	O	0.32667000	-1.90009000	-2.93623000
O	0.14820000	-2.97459000	-0.97261000	O	0.87667000	-2.42009000	-0.90623000
C	1.64820000	-6.69459000	-3.39261000	C	3.33667000	-5.61009000	-3.21623000
O	0.96893727	-7.72732968	-3.62845203	O	3.38255009	-6.85196758	-3.41423415
N	-0.70180000	6.61541000	2.79739000	N	-2.73333000	5.52991000	3.44377000
H	0.23590841	6.26837064	2.81371886	H	-1.78965485	5.46981323	3.76913992
C	-1.56180000	5.65540000	2.12739000	C	-3.32333000	4.41991000	2.72377000
H	-2.30180000	6.23541000	1.57739000	H	-4.34333000	4.63991000	2.44377000
C	-0.87180000	4.84541000	1.02739000	C	-2.49333000	4.14991000	1.46377000
H	-0.24180000	5.48541000	0.41739000	H	-2.52333000	5.09991000	0.92377000
H	-0.20180000	4.10541000	1.46739000	H	-1.47334000	4.03991000	1.82377000
C	-1.77180000	4.04540000	0.12739000	C	-3.05333000	3.17991000	0.46377000
N	-1.73180000	2.65540000	-0.01261000	N	-2.56334000	1.88991000	0.28377000
C	-2.75180000	4.54540000	-0.69261000	C	-4.20333000	3.24991000	-0.27623000
H	-3.03180000	5.57541000	-0.85261000	H	-4.89333000	4.07991000	-0.39623000
C	-2.69180000	2.38540000	-0.90261000	C	-3.41333000	1.25991000	-0.53623000
H	-3.07180000	1.44541000	-1.27261000	H	-3.37333000	0.22991000	-0.86623000
N	-3.28180000	3.48541000	-1.39261000	N	-4.37333000	2.07991000	-0.98623000
H	-3.96180000	3.48541000	-2.13261000	H	-5.12333000	1.80991000	-1.59623000
C	-2.15180000	4.93541000	3.33739000	C	-3.37333000	3.24991000	3.69377000
O	-1.43267083	4.16199012	4.02167466	O	-2.37208800	2.49922729	3.82628598
N	-4.04180000	1.97540000	4.83739000	N	-4.07333000	-0.14009000	4.95377000
H	-3.13343202	2.07084835	5.24452293	H	-3.48180130	-0.04845145	5.75482941
C	-4.55180000	0.65540000	4.49739000	C	-4.17333000	-1.54009000	4.58377000
H	-5.10180000	0.69541000	3.55739000	H	-4.82333000	-1.68009000	3.71377000
C	-3.33180000	-0.25460000	4.30739000	C	-2.77333000	-2.08009000	4.28377000
H	-2.55180000	0.01540000	5.01739000	H	-2.07333000	-1.81009000	5.06377000
H	-3.55180000	-1.31459000	4.45739000	H	-2.87333000	-3.16009000	4.34377000
C	-2.86180000	-0.27460000	2.87739000	C	-2.13333000	-1.67009000	2.98377000
N	-3.17180000	-1.30459000	2.01739000	N	-2.25333000	-2.43009000	1.83377000
H	-3.79180000	-2.07460000	2.24739000	H	-2.65334000	-3.35009000	1.73377000
C	-1.94180000	0.50541000	2.22739000	C	-1.55333000	-0.50009000	2.58377000
H	-1.46180000	1.37541000	2.64739000	H	-1.32333000	0.35991000	3.19377000
C	-2.58180000	-1.04459000	0.84739000	C	-1.69333000	-1.72009000	0.83377000
H	-2.54180000	-1.58459000	-0.09261000	H	-1.54333000	-2.11009000	-0.16623000
N	-1.79180000	0.02541000	0.92739000	N	-1.25333000	-0.52009000	1.22377000
C	-5.42180000	0.12541000	5.62739000	C	-4.76333000	-2.34009000	5.73377000
O	-5.15701250	0.42731843	6.81999615	O	-4.51427530	-2.01057203	6.92245004
Cu	-0.43180000	1.08540000	-0.12261000	Cu	-0.69333000	1.08991000	-0.00623000
O	-1.74180000	1.72540000	-3.84261000	O	1.24667000	4.30991000	1.07377000
H	-0.99180000	1.56540000	-4.41261000	H	0.92667000	4.85991000	0.36377000
H	-2.49180000	1.71541000	-4.42261000	H	2.09666000	4.68991000	1.30377000
O	0.39820000	-1.65459000	2.64739000	O	1.37667000	-3.52009000	1.34377000
H	1.32820000	-1.56459000	2.85739000	H	2.07667000	-2.89009000	1.49377000
H	0.31820000	-2.54459000	2.30739000	H	1.10667000	-3.36009000	0.43377000
O	4.18820000	3.34541000	3.45739000	O	0.19667000	5.44991000	3.73377000
H	5.09820000	3.64541000	3.43739000	H	0.58667000	4.91991000	3.03377000

H	3.89820000	3.39541000	2.54739000	H	0.60667000	6.30991000	3.64377000
O	-4.68180000	-0.75460000	-1.60261000	O	2.60667000	-1.96009000	-4.11623000
H	-4.92180000	-0.82460000	-2.53261000	H	2.67667000	-1.23009000	-4.73623000
H	-4.48180000	-1.65459000	-1.34261000	H	1.71667000	-1.89009000	-3.76623000
O	2.67820000	3.79540000	1.25739000	O	-4.33333000	-1.93009000	-1.58623000
H	3.23820000	3.87541000	0.48739000	H	-3.83333000	-2.74009000	-1.54623000
H	2.63820000	4.68541000	1.61739000	H	-4.54333000	-1.83009000	-2.51623000
O	3.67820000	-1.57460000	3.52739000	O	1.19667000	-2.27009000	4.06377000
H	3.83820000	-1.46459000	2.59739000	H	1.12667000	-2.71009000	3.22377000
H	4.23820000	-2.30459000	3.78739000	H	2.05667000	-2.53009000	4.39377000
O	-0.22180000	-4.17459000	1.42739000	O	3.78667000	-2.31009000	1.70377000
H	0.21820000	-3.81459000	0.65739000	H	4.57667000	-2.82009000	1.51377000
H	0.33820000	-4.89459000	1.71739000	H	4.06667000	-1.40009000	1.64377000
O	-1.19180000	-0.12459000	-1.89261000	O	-2.51333000	0.75991000	-4.13623000
H	-0.91180000	-0.97459000	-2.24261000	H	-3.25333000	0.13991000	-4.11623000
H	-1.52180000	0.34541000	-2.66261000	H	-1.82333000	0.29991000	-4.60623000
O	1.79820000	0.59541000	-5.37261000	O	-1.11333000	-0.11009000	-1.83623000
H	0.89820000	0.31540000	-5.25261000	H	-0.55333000	-0.77009000	-2.24623000
H	2.26820000	0.23541000	-4.62261000	H	-1.77333000	0.09991000	-2.50623000
O	0.76820000	1.64541000	1.61739000	O	-0.36333000	-0.69009000	-5.28623000
H	1.38820000	2.31540000	1.32739000	H	-0.23333000	-1.30009000	-4.55623000
H	0.74820000	1.72540000	2.56739000	H	0.45667000	-0.72009000	-5.76623000
O	-0.69180000	-0.90459000	-5.24261000	O	0.08667000	1.86991000	1.95377000
H	-1.64180000	-0.84460000	-5.34261000	H	0.60667000	1.31991000	2.55377000
H	-0.56180000	-1.44459000	-4.46261000	H	0.67667000	2.58991000	1.72377000
O	0.88820000	1.93541000	4.45739000	O	1.72667000	6.21991000	-1.14623000
H	0.27820000	1.51540000	5.06739000	H	2.65667000	6.34991000	-1.31623000
H	1.69820000	1.45541000	4.54739000	H	1.30667000	6.30991000	-1.99623000
H	-6.25881162	-0.50403775	5.40805673	O	1.80667000	0.31991000	3.33377000
H	2.30994129	-6.30747879	-4.13903038	H	2.75667000	0.21991000	3.26377000
H	-3.17679194	5.08840275	3.60363189	H	1.49667000	-0.52009000	3.69377000
H	-0.72667120	7.48555595	2.30522392	H	3.59933291	-4.93298534	-4.00200190
H	-4.59974148	2.78693790	4.66387474	H	-4.25985504	3.06492509	4.26364186
				H	-3.26973069	6.35623499	3.61541298
				H	-4.98353398	0.21355612	5.16932308
				H	-5.39040872	-3.18340806	5.53255635
Frame 7:				Frame 8:			
N	1.26614000	0.08386000	-0.74140000	N	1.01683000	-0.81100000	0.35667000
H	1.22614000	-0.83614000	-0.31140000	H	0.26683000	-1.39100000	0.68667000
H	2.12614000	0.44386000	-0.35141000	H	1.69683000	-0.96100000	1.08667000
C	1.77614000	-0.48614000	-1.96140000	C	1.63683000	-1.73100000	-0.57333000
H	1.06614000	-1.17614000	-2.41140000	H	0.92683000	-2.21100000	-1.25333000
C	1.94614000	0.63386000	-3.00140000	C	2.78683000	-1.06100000	-1.32333000
H	2.60614000	1.42386000	-2.63140000	H	3.51683000	-0.64100000	-0.63334000
H	2.33614000	0.24386000	-3.94141000	H	3.31684000	-1.79100000	-1.93333000
C	0.62614000	1.15386000	-3.50140000	C	2.23683000	-0.10100000	-2.35333000
N	-0.35386000	1.74386000	-2.71140000	N	1.46683000	1.01900000	-2.07333000
C	0.14614000	1.01386000	-4.77140000	C	2.57683000	0.02900000	-3.67333000
H	0.60614000	0.54386000	-5.63140000	H	3.25683000	-0.60100000	-4.23333000
C	-1.37386000	1.96386000	-3.55140000	C	1.20683000	1.61900000	-3.23333000
H	-2.26386000	2.46386000	-3.20140000	H	0.54683000	2.46900000	-3.38334000
N	-1.13386000	1.54386000	-4.80140000	N	1.93683000	1.10900000	-4.23333000
H	-1.84386000	1.43386000	-5.50140000	H	1.90684000	1.23900000	-5.23333000
C	3.06614000	-1.24614000	-1.68140000	C	2.22684000	-2.78100000	0.34667000
O	4.01614000	-0.70614000	-1.11140000	O	2.85683000	-2.37100000	1.32667000
N	3.16614000	-2.54614000	-1.93140000	N	1.91683000	-4.06100000	0.12667000
H	2.30614000	-3.02614000	-2.18140000	H	1.34683000	-4.24100000	-0.68333000
C	4.22614000	-3.52614000	-1.77140000	C	2.23683000	-5.07100000	1.12667000
H	4.54614000	-3.89614000	-2.75140000	H	2.99683000	-5.80100000	0.85667000
H	5.06614000	-2.99614000	-1.33140000	H	2.55683000	-4.57100000	2.04667000
C	3.86614000	-4.62614000	-0.78141000	C	0.97684000	-5.82100000	1.54667000
O	4.52614000	-5.65614000	-0.91140000	O	1.08683000	-7.00100000	1.86666000
N	2.94614000	-4.39614000	0.15860000	N	-0.18316000	-5.18100000	1.52666000
H	2.47614000	-3.51614000	0.33860000	H	-0.14317000	-4.21100000	1.23667000
C	2.45614000	-5.39614000	1.07860000	C	-1.46317000	-5.75100000	1.91667000
H	3.40614000	-5.67614000	1.54860000	H	-1.26317000	-6.02100000	2.95666000
C	1.47614000	-4.79614000	2.07860000	C	-2.51317000	-4.66100000	2.08667000

H	1.13614000	-5.54614000	2.78860000	H	-3.46317000	-5.07100000	2.43667000
H	1.98614000	-3.99614000	2.62860000	H	-2.35317000	-3.96100000	2.91667000
C	0.16614000	-4.23614000	1.51860000	C	-2.73317000	-3.86100000	0.80667000
H	-0.34386000	-5.10614000	1.09860000	H	-2.43316000	-4.51100000	-0.02333000
H	-0.41386000	-3.82614000	2.33860000	H	-3.81317000	-3.76100000	0.68667000
C	0.35614000	-3.03614000	0.58860000	C	-1.95317000	-2.56100000	0.76667000
O	-0.45386000	-2.84614000	-0.34140000	O	-2.49317000	-1.52100000	0.30667000
O	1.40614000	-2.37614000	0.74860000	O	-0.83317000	-2.47100000	1.29667000
C	1.93614000	-6.72614000	0.54860000	C	-2.07317000	-6.96100000	1.23667000
O	1.70377203	-7.67296967	1.34426907	O	-3.00471394	-7.59474876	1.79716885
N	-0.39386000	6.98386000	-0.45140000	N	3.42683000	6.21900000	-1.41333000
H	0.53486474	6.76666087	-0.75189110	H	4.10249292	5.55588363	-1.09121776
C	-1.26386000	5.93386000	0.01860000	C	2.11683000	5.87900000	-0.87333000
H	-2.31386000	6.23386000	0.07860000	H	1.36683000	6.58900000	-1.21333000
C	-1.21386000	4.78386000	-0.97140000	C	1.62683000	4.53900000	-1.41333000
H	-1.45386000	5.15386000	-1.96140000	H	1.47684000	4.46900000	-2.49333000
H	-0.30386000	4.18386000	-1.12140000	H	2.36683000	3.75900000	-1.22334000
C	-2.25386000	3.70386000	-0.81140000	C	0.19683000	4.16900000	-1.15333000
N	-2.04386000	2.33386000	-0.64140000	N	-0.20317000	2.91900000	-0.70333000
C	-3.59386000	3.96386000	-0.76140000	C	-0.86317000	4.89900000	-1.64333000
H	-4.22386000	4.80386000	-1.00140000	H	-0.86317000	5.86900000	-2.11333000
C	-3.26386000	1.80386000	-0.52140000	C	-1.51317000	2.95900000	-0.92333000
H	-3.41386000	0.74386000	-0.37140000	H	-2.25317000	2.22900000	-0.61333000
N	-4.20386000	2.75386000	-0.48140000	N	-1.97317000	4.13900000	-1.36333000
H	-5.19386000	2.55386000	-0.55140000	H	-2.95317000	4.32900000	-1.52333000
C	-0.83386000	5.49386000	1.40860000	C	2.22684000	5.68900000	0.63667000
O	0.21063403	4.80773517	1.55636837	O	2.72147240	4.63011009	1.10321208
N	-1.21386000	3.45386000	4.76860000	N	0.84683000	5.09900000	3.96667000
H	-0.38526215	3.74854937	5.24460818	H	1.71988235	4.65777299	3.75906865
C	-1.72386000	2.24386000	5.38860000	C	-0.09316000	4.45900000	4.86666000
H	-2.77386000	2.08386000	5.15860000	H	-1.08317000	4.55900000	4.43667000
C	-0.90386000	1.02386000	4.98860000	C	0.29683000	2.97900000	4.85667000
H	0.09614000	1.23386000	5.36860000	H	1.37683000	2.88900000	4.95666000
H	-1.14386000	0.07386000	5.48860000	H	0.03683000	2.49900000	5.80667000
C	-0.89386000	0.68386000	3.52860000	C	-0.18316000	2.23900000	3.64667000
N	-1.49386000	-0.47614000	3.08860000	N	-1.20317000	1.30900000	3.66667000
H	-1.88386000	-1.18614000	3.68860000	H	-1.80317000	1.06900000	4.43667000
C	-0.41386000	1.27386000	2.37860000	C	0.19683000	2.24900000	2.32667000
H	0.11614000	2.20386000	2.26860000	H	0.95683000	2.84900000	1.83667000
C	-1.45386000	-0.46614000	1.73860000	C	-1.33317000	0.77900000	2.44667000
H	-1.85386000	-1.21614000	1.06860000	H	-1.97317000	-0.06100000	2.21667000
N	-0.80386000	0.58386000	1.23860000	N	-0.43316000	1.25900000	1.57667000
C	-1.56386000	2.41386000	6.89859000	C	0.03683000	5.03900000	6.26667000
O	-0.72416593	3.23302151	7.35406652	O	1.13769976	5.51104617	6.65245328
Cu	-0.43386000	1.18386000	-0.68140000	Cu	0.57683000	1.08900000	-0.19333000
O	5.81614000	0.25386000	0.86860000	O	0.07683000	-1.91100000	3.92667000
H	6.09614000	-0.33614000	1.56860000	H	0.71683000	-2.57100000	4.19667000
H	5.15614000	-0.24614000	0.39859000	H	-0.17317000	-2.17100000	3.04667000
O	-4.20386000	1.01386000	-4.22140000	O	-0.37317000	-4.33100000	-1.85333000
H	-4.89386000	0.80386000	-3.59140000	H	-1.22317000	-4.12100000	-2.22334000
H	-3.70386000	0.20386000	-4.31140000	H	0.25683000	-3.99100000	-2.49333000
O	-3.09386000	-3.35614000	0.09860000	O	2.28683000	-0.02100000	2.80667000
H	-3.22386000	-3.75614000	0.95860000	H	1.61683000	-0.11100000	3.48667000
H	-2.15386000	-3.17614000	0.05859000	H	3.07683000	-0.37100000	3.21667000
O	3.01614000	0.39386000	3.70860000	O	-4.10317000	1.91900000	1.06667000
H	3.80614000	0.51386000	4.24860000	H	-4.35317000	1.00900000	1.23667000
H	3.26614000	-0.24614000	3.04860000	H	-4.66317000	2.17900000	0.32667000
O	2.08614000	5.23386000	-1.30140000	O	-5.10317000	2.11900000	-1.44333000
H	2.31614000	5.62386000	-2.15140000	H	-4.30317000	1.90900000	-1.91333000
H	2.23614000	4.29386000	-1.42140000	H	-5.81317000	1.72900000	-1.95333000
O	-5.98386000	0.36386000	-2.44141000	O	4.57683000	3.89900000	-2.29334000
H	-6.92386000	0.53386000	-2.36140000	H	4.31684000	2.98900000	-2.46333000
H	-5.74386000	-0.04614000	-1.61140000	H	5.36683000	4.02900000	-2.82333000
O	-4.99386000	-1.09614000	1.18860000	O	1.61683000	-3.43100000	-3.61333000
H	-5.82386000	-1.36614000	0.78860000	H	2.01683000	-3.98100000	-4.27333000
H	-4.40386000	-1.82614000	0.99860000	H	1.36683000	-2.63100000	-4.09333000
O	3.68614000	-1.49614000	1.85860000	O	-1.25317000	-0.04100000	-1.47334000

H	4.24614000	-2.26614000	1.84860000	H	-1.83317000	-0.65100000	-1.03333000
H	2.81614000	-1.83614000	1.64859000	H	-0.88317000	-0.54100000	-2.20333000
O	-1.45386000	-0.66614000	-1.34140000	O	5.49683000	-2.77100000	1.86666000
H	-1.01386000	-1.48614000	-1.09140000	H	4.57683000	-2.53100000	1.76667000
H	-2.14386000	-0.94614000	-1.95140000	H	5.78683000	-2.97100000	0.97667000
O	3.31614000	1.43386000	1.05859000	O	-4.02316000	-2.50100000	-1.74333000
H	3.17614000	1.02386000	1.91860000	H	-4.94317000	-2.24100000	-1.67333000
H	4.22614000	1.24386000	0.84860000	H	-3.59316000	-2.03100000	-1.03333000
O	1.12614000	2.86386000	0.12860000	O	-0.57317000	-1.38100000	-3.95333000
H	1.98614000	2.56386000	0.41860000	H	-1.19317000	-2.11100000	-3.93333000
H	0.86614000	3.52386000	0.76860000	H	-0.85317000	-0.85100000	-4.70333000
O	0.81614000	-3.86614000	-2.56140000	O	-3.48317000	1.49900000	-3.54334000
H	0.12614000	-3.97614000	-3.21140000	H	-4.12317000	0.91900000	-3.95333000
H	0.35614000	-3.66614000	-1.74140000	H	-3.63317000	2.34900000	-3.95333000
O	-3.21386000	-1.62614000	-2.91140000	O	2.59683000	1.76900000	0.37667000
H	-2.75386000	-2.19614000	-3.54140000	H	3.07683000	2.59900000	0.31667000
H	-4.05386000	-2.06614000	-2.76140000	H	2.94683000	1.35900000	1.17667000
H	-2.16579315	1.83638834	7.56874145	O	-4.89317000	-0.57100000	1.22667000
H	-1.90502228	4.17432199	4.82542624	H	-5.43316000	-0.37100000	0.45666000
H	-1.41929447	5.76753895	2.26139911	H	-4.11317000	-0.98100000	0.87667000
H	-0.71939177	7.92905064	-0.47677176	O	-1.24317000	1.16900000	-5.22334000
H	1.76844050	-6.85533457	-0.50024968	H	-1.87317000	1.16900000	-4.51333000
Frame 9:				Frame 10:			
N	-0.26619000	-1.14762000	0.57349000	N	-0.18965000	-0.66035000	-1.22868000
H	-0.89619000	-0.71762000	1.23349000	H	-0.69965000	-1.27035000	-0.59869000
H	0.43381000	-1.51762000	1.19349000	H	0.29035000	-1.37035000	-1.76868000
C	-1.03619000	-2.32762000	0.24349000	C	-1.25965000	-0.37035000	-2.15868000
H	-2.09619000	-2.22762000	0.01349000	H	-2.06965000	0.26965000	-1.79868000
C	-0.37619000	-3.01762000	-0.95651000	C	-0.65965000	0.46965000	-3.27869000
H	0.62381000	-3.41762000	-0.75651000	H	0.29035000	-0.01035000	-3.51868000
H	-0.94619000	-3.88762000	-1.24651000	H	-1.22965000	0.42965000	-4.20868000
C	-0.40619000	-2.24762000	-2.24651000	C	-0.23965000	1.85965000	-2.87868000
N	0.13381000	-0.97762000	-2.43651000	N	0.38035000	2.09965000	-1.64869000
C	-0.85619000	-2.74762000	-3.43651000	C	-0.33965000	3.00965000	-3.60868000
H	-1.25619000	-3.72762000	-3.66651000	H	-0.86965000	3.02965000	-4.54868000
C	0.00381000	-0.78762000	-3.74651000	C	0.53035000	3.41965000	-1.69868000
H	0.30381000	0.11238000	-4.26651000	H	0.88035000	4.02965000	-0.87868000
N	-0.58619000	-1.79762000	-4.40651000	N	0.11035000	4.03965000	-2.80868000
H	-0.75619000	-1.85762000	-5.40651000	H	0.08035000	5.04965000	-2.88868000
C	-1.18619000	-3.16762000	1.50349000	C	-1.89965000	-1.64035000	-2.68869000
O	-0.20619000	-3.32762000	2.22349000	O	-1.23965000	-2.60035000	-3.09869000
N	-2.38619000	-3.72762000	1.70349000	N	-3.21965000	-1.74035000	-2.50869000
H	-3.19619000	-3.46762000	1.15349000	H	-3.70965000	-0.92035000	-2.17868000
C	-2.61619000	-4.43762000	2.93349000	H	-4.16965000	-2.75035000	-2.90868000
H	-2.95619000	-5.43762000	2.65349000	C	-4.77965000	-2.29035000	-3.68869000
H	-1.75619000	-4.48762000	3.60349000	H	-3.54965000	-3.55035000	-3.29868000
C	-3.72619000	-3.77762000	3.75349000	C	-4.95965000	-3.40035000	-1.76868000
O	-4.48619000	-4.34762000	4.53349000	O	-6.01965000	-3.95035000	-2.04868000
N	-3.67619000	-2.44762000	3.71349000	N	-4.42965000	-3.35035000	-0.54868000
H	-2.86619000	-2.03762000	3.27349000	H	-3.50965000	-2.93035000	-0.51868000
C	-4.59619000	-1.57762000	4.42349000	C	-5.01965000	-3.85035000	0.67131000
H	-4.50619000	-1.86762000	5.46349000	H	-5.23965000	-4.90035000	0.54132000
C	-4.14619000	-0.11762000	4.25349000	C	-3.87965000	-3.76035000	1.68132000
H	-4.70619000	0.55238000	4.90349000	H	-4.09965000	-4.40035000	2.53132000
H	-3.13619000	0.04238000	4.63349000	H	-3.09965000	-4.33035000	1.17131000
C	-4.26619000	0.44238000	2.83349000	C	-3.43965000	-2.38035000	2.16132000
H	-5.11619000	0.04238000	2.28349000	H	-4.28965000	-1.78035000	2.49131000
H	-4.40619000	1.51238000	2.98349000	H	-2.93965000	-2.43035000	3.13131000
C	-3.04619000	0.45238000	1.93349000	C	-2.78965000	-1.54035000	1.07132000
O	-3.07619000	0.98238000	0.80349000	O	-3.01965000	-0.31035000	1.00132000
O	-1.97619000	0.00238000	2.39349000	O	-1.89965000	-2.10035000	0.39132000

C	-6.05619000	-1.69762000	4.01349000	C	-6.35965000	-3.24035000	1.09132000
O	-6.95300877	-1.16319607	4.71611203	O	-6.93647280	-3.64589373	2.13361569
N	6.39381000	0.62238000	-3.11651000	N	6.66035000	2.48965000	-1.07869000
H	6.58714958	-0.13051610	-2.48740963	H	6.60740550	1.79581633	-1.79687641
C	5.25381000	1.48238000	-2.88651000	C	5.56035000	2.64965000	-0.13868000
H	5.11381000	2.15238000	-3.73651000	H	5.71035000	3.58965000	0.39132000
C	3.96381000	0.67238000	-2.74651000	C	4.15035000	2.50965000	-0.71868000
H	3.97381000	-0.04762000	-3.56651000	H	4.10035000	3.11965000	-1.61869000
H	4.00381000	0.13238000	-1.79651000	H	4.19035000	1.44965000	-0.95868000
C	2.66381000	1.42238000	-2.84651000	C	3.09035000	2.86965000	0.29132000
N	1.56381000	1.44238000	-1.98651000	N	2.03035000	2.04965000	0.65131000
C	2.47381000	2.24238000	-3.91651000	C	3.06035000	4.03965000	0.99131000
H	3.10381000	2.36238000	-4.78651000	H	3.74035000	4.86965000	0.85131000
C	0.76381000	2.37238000	-2.51651000	C	1.35035000	2.72965000	1.59132000
H	-0.00619000	2.76238000	-1.86651000	H	0.39035000	2.42965000	1.98132000
N	1.30381000	2.91238000	-3.61651000	N	1.93035000	3.92965000	1.77132000
H	0.93381000	3.69238000	-4.14651000	H	1.52035000	4.66965000	2.32132000
C	5.48381000	2.21238000	-1.57651000	C	5.78035000	1.48965000	0.82132000
O	5.32437068	1.60918664	-0.48366626	O	5.47361428	0.31939921	0.47491438
N	4.75381000	4.27238000	1.29349000	N	5.35035000	-0.62035000	3.79132000
H	4.80828145	3.28414103	1.43637666	H	5.51631952	-1.03835071	2.91019960
C	3.80381000	4.84238000	2.22349000	C	4.31035000	-1.12035000	4.66132000
H	3.03381000	5.43238000	1.73349000	H	3.69035000	-0.32035000	5.07132000
C	3.13381000	3.68238000	2.96349000	C	3.30035000	-1.99035000	3.92131000
H	3.86381000	2.98238000	3.37349000	H	3.88035000	-2.69035000	3.31131000
H	2.50381000	4.10238000	3.73349000	H	2.67035000	-2.63035000	4.54132000
C	2.24381000	2.84238000	2.07349000	C	2.34035000	-1.28035000	3.01131000
N	0.97381000	3.25238000	1.73349000	N	1.06035000	-0.91035000	3.40131000
H	0.56381000	4.07238000	2.15349000	H	0.60035000	-1.06035000	4.28132000
C	2.36381000	1.63238000	1.45349000	C	2.40035000	-0.98035000	1.68132000
H	3.28381000	1.08238000	1.38349000	H	3.23035000	-0.97035000	0.98132000
C	0.34381000	2.23238000	1.12349000	C	0.32035000	-0.70035000	2.30132000
H	-0.68619000	2.27238000	0.80349000	H	-0.69965000	-0.35035000	2.32132000
N	1.18381000	1.24238000	0.81349000	N	1.12035000	-0.64035000	1.23132000
C	4.60381000	5.60238000	3.26349000	C	4.91035000	-2.00035000	5.75132000
O	5.71481582	5.15689050	3.65178850	O	5.71940382	-2.91498176	5.44726208
Cu	0.63381000	0.06238000	-0.70651000	Cu	0.83035000	0.67965000	-0.28868000
O	2.11381000	-5.04762000	1.28349000	O	1.90035000	-4.77035000	0.68132000
H	1.42381000	-4.83762000	1.91349000	H	1.03035000	-4.62035000	0.31131000
H	1.65381000	-5.48762000	0.57349000	H	2.13035000	-5.66035000	0.41132000
O	2.24381000	-1.57762000	2.39349000	O	-4.75965000	0.07965000	-0.82869000
H	1.80381000	-2.35762000	2.72349000	H	-5.00965000	0.99965000	-0.78868000
H	2.94381000	-1.40762000	3.02349000	H	-4.14965000	-0.04035000	-0.09869000
O	-1.91619000	1.42238000	-4.13651000	O	4.96035000	-1.93035000	-1.95868000
H	-2.51619000	1.23238000	-4.85651000	H	4.49035000	-1.86035000	-2.78868000
H	-2.11619000	2.31238000	-3.87651000	H	4.53035000	-1.29035000	-1.38868000
O	1.18381000	-4.89762000	-3.09651000	O	-3.49965000	1.04965000	3.19132000
H	0.57381000	-5.47762000	-3.55651000	H	-3.71965000	1.93965000	2.93132000
H	0.96381000	-4.98762000	-2.16651000	H	-3.17965000	0.62965000	2.39132000
O	-4.15619000	0.06238000	-2.65651000	O	-0.63965000	6.37965000	-0.19868000
H	-3.52619000	0.73238000	-2.91651000	H	-1.31965000	5.73965000	0.03132000
H	-5.00619000	0.40238000	-2.94651000	H	-1.01965000	7.22965000	0.03132000
O	-2.09619000	4.07238000	-3.24651000	O	1.53035000	-2.24035000	-2.89869000
H	-2.98619000	3.99238000	-3.59651000	H	1.86035000	-3.10035000	-2.63868000
H	-1.61619000	4.55238000	-3.91651000	H	0.81035000	-2.44035000	-3.49868000
O	-0.08619000	-0.86762000	4.23349000	O	-1.36965000	1.43965000	0.39132000
H	0.76381000	-0.80762000	3.78349000	H	-2.09965000	0.80965000	0.43132000
H	-0.71619000	-0.58762000	3.57349000	H	-1.76965000	2.26965000	0.64132000
O	3.00381000	-2.86762000	-2.59651000	O	-1.04965000	1.96965000	3.92131000
H	3.67381000	-3.48762000	-2.28651000	H	-1.30965000	2.88965000	3.92131000
H	2.32381000	-3.42762000	-2.96651000	H	-1.86965000	1.47965000	3.96132000
O	-3.79619000	3.62238000	0.57349000	O	-3.47965000	2.38965000	-3.17868000
H	-4.34619000	3.70238000	-0.20651000	H	-3.60965000	2.50965000	-2.23869000
H	-3.30619000	2.81238000	0.44349000	H	-3.71965000	1.47965000	-3.34869000
O	-5.44619000	-0.13762000	-0.18651000	O	2.52035000	0.01965000	-1.82869000
H	-4.70619000	0.13238000	0.35349000	H	2.94035000	0.64965000	-2.40868000
H	-5.09619000	-0.14762000	-1.07651000	H	2.19035000	-0.66035000	-2.40868000

O	5.26381000	-0.32762000	1.14349000	O	3.46035000	1.61965000	-3.67868000
H	5.17381000	0.13238000	1.98349000	H	3.18035000	1.59965000	-4.59869000
H	5.36381000	0.38238000	0.50349000	H	4.42035000	1.61965000	-3.71868000
O	-1.50619000	0.92238000	-1.10651000	O	-0.84965000	-4.40035000	-0.21868000
H	-2.23619000	0.92238000	-0.48651000	H	-1.63965000	-4.81035000	-0.56868000
H	-1.89619000	0.62238000	-1.92651000	H	-1.12965000	-3.53035000	0.07132000
O	6.73381000	-1.34762000	-1.22651000	O	-2.15965000	4.01965000	0.69132000
H	6.56381000	-2.25762000	-1.43651000	H	-2.87965000	4.49965000	0.26131000
H	6.14381000	-1.14762000	-0.49651000	H	-2.15965000	4.34965000	1.59132000
O	-1.62619000	4.76238000	-0.56651000	H	-6.80566824	-2.46921255	0.49860189
H	-2.38619000	4.64238000	0.01349000	H	6.19585754	1.66903639	1.79089414
H	-1.95619000	4.54238000	-1.43651000	H	7.46891684	3.07357496	-1.00622409
O	2.47381000	-1.17762000	-0.58651000	H	5.87322244	0.19037611	4.05410891
H	2.92381000	-1.49762000	0.19349000	H	4.64368953	-1.84050923	6.77515745
H	2.65381000	-1.82762000	-1.26651000				
O	-3.82619000	-2.05762000	-4.42651000				
H	-4.61619000	-1.75762000	-4.88651000				
H	-3.75619000	-1.45762000	-3.67651000				
O	-1.60619000	2.32238000	3.91349000				
H	-0.77619000	2.61238000	3.53349000				
H	-1.75619000	1.46238000	3.52349000				
H	4.22366509	6.51747500	3.66721142				
H	4.45594112	4.45786869	0.35707766				
H	5.78158558	3.24009640	-1.58186773				
H	6.98862905	0.78070029	-3.90462483				
H	-6.32057868	-2.23643936	3.12767268				
Frame 11:				Frame 12:			
N	-0.34733000	-0.97358000	-0.22441000	N	-0.44184	-0.99062	-0.49380
H	-0.98733000	-0.94358000	0.55558000	H	-1.12184	-0.73062	0.20620
H	0.10267000	-1.80358000	0.15558000	H	0.00816	-1.81062	-0.13380
C	-1.33733000	-1.38359000	-1.19442000	C	-1.21184	-1.57062	-1.57380
H	-2.07733000	-0.59358000	-1.11442000	H	-2.06184	-0.98062	-1.91380
C	-0.77733000	-1.39358000	-2.62442000	C	-0.23184	-1.89062	-2.71380
H	-0.01733000	-2.11358000	-2.88441000	H	0.64816	-2.44062	-2.37380
H	-1.60733000	-1.69358000	-3.27442000	H	-0.79184	-2.47062	-3.44380
C	-0.55733000	0.01642000	-3.11442000	C	0.08816	-0.63062	-3.46380
N	0.28267000	0.87642000	-2.41442000	N	0.61816	0.46938	-2.79380
C	-1.15733000	0.60642000	-4.19442000	C	-0.18184	-0.30062	-4.77380
H	-1.83733000	0.10642000	-4.86442000	H	-0.55184	-0.81062	-5.64380
C	0.17267000	1.98642000	-3.14442000	C	0.56816	1.45938	-3.68380
H	0.62266000	2.89642000	-2.79441000	H	0.87816	2.46938	-3.47380
N	-0.55733000	1.84642000	-4.26442000	N	0.08816	1.04938	-4.87380
H	-0.81733000	2.61641000	-4.87442000	H	-0.12184	1.63938	-5.66380
C	-1.89733000	-2.70359000	-0.68442000	C	-1.79184	-2.88062	-1.07380
O	-1.10733000	-3.60358000	-0.41442000	O	-1.04184	-3.72062	-0.58380
N	-3.21733000	-2.86358000	-0.54441000	N	-3.13184	-2.93062	-0.98380
H	-3.75733000	-2.10358000	-0.94442000	H	-3.54184	-2.10062	-1.37380
C	-3.91733000	-3.95359000	0.10558000	C	-4.03184	-4.00062	-0.61380
H	-4.76733000	-4.29359000	-0.48442000	H	-4.62184	-4.36062	-1.45380
H	-3.31733000	-4.79359000	0.44558000	H	-3.40184	-4.82062	-0.29380
C	-4.61733000	-3.52358000	1.38558000	C	-4.97184	-3.57062	0.50620
O	-5.09733000	-4.41358000	2.08558000	O	-5.90184	-4.30062	0.82620
N	-4.60733000	-2.24358000	1.75558000	N	-4.71184	-2.49062	1.24620
H	-4.07733000	-1.64358000	1.13558000	H	-3.91184	-1.91062	1.04620
C	-5.22733000	-1.73358000	2.95559000	C	-5.46184	-1.95062	2.36620
H	-5.60733000	-2.64358000	3.43558000	H	-5.51184	-2.73062	3.12620
C	-4.24733000	-1.05358000	3.90558000	C	-4.55184	-0.88062	2.96620
H	-4.73733000	-0.97358000	4.87558000	H	-5.02184	-0.46062	3.85620
H	-3.46733000	-1.79359000	4.07558000	H	-3.60184	-1.29062	3.30620
C	-3.61733000	0.28642000	3.50558000	C	-4.23184	0.32938	2.08620
H	-4.40733000	1.01642000	3.31558000	H	-5.12184	0.74938	1.60620
H	-2.99733000	0.74642000	4.27559000	H	-4.00184	1.12938	2.78620
C	-2.78734000	0.31642000	2.23558000	C	-3.19184	0.20938	0.97620
O	-2.63733000	1.39642000	1.63558000	O	-3.32184	0.93938	-0.03380
O	-2.26733000	-0.74358000	1.81558000	O	-2.32184	-0.65062	1.19620
C	-6.48733000	-0.91358000	2.71558000	C	-6.83184	-1.43062	1.98620
O	-7.11910772	-0.43074291	3.69092395	O	-7.73628	-1.34539	2.85700

N	5.95267000	2.01642000	-3.55442000	N	6.50816	0.64938	-3.13380
H	5.80224875	1.04032977	-3.71133178	H	5.93115	-0.03919	-3.57303
C	5.21266000	2.43642000	-2.38441000	C	5.73816	1.34938	-2.11380
H	5.53267000	3.46642000	-2.26442000	H	6.06816	2.34938	-1.85380
C	3.70267000	2.29641000	-2.60442000	C	4.26816	1.39938	-2.55380
H	3.44267000	2.85642000	-3.50442000	H	4.22816	1.90938	-3.51380
H	3.49267000	1.27642000	-2.92442000	H	3.91816	0.36938	-2.65380
C	2.78267000	2.82642000	-1.54441000	C	3.42816	2.30938	-1.71380
N	2.09267000	2.07642000	-0.59442000	N	2.32816	1.91938	-0.94380
C	2.58267000	4.16642000	-1.34442000	C	3.61816	3.65938	-1.61380
H	2.98267000	5.03642000	-1.84442000	H	4.34816	4.29938	-2.08380
C	1.58267000	2.97642000	0.24558000	C	1.88816	3.04938	-0.39380
H	0.93267000	2.75642000	1.07558000	H	1.02816	3.21938	0.24620
N	1.71266000	4.20641000	-0.27442000	N	2.50816	4.11938	-0.92380
H	1.25267000	5.03642000	0.09558000	H	2.24816	5.06938	-0.70380
C	5.61267000	1.56642000	-1.20442000	C	5.86816	0.50938	-0.85380
O	4.96556187	0.51814343	-0.94763631	O	5.23126	-0.57090	-0.74929
N	6.18267000	0.48642000	2.26558000	N	5.39816	-0.03062	3.21620
H	6.70182859	-0.35169745	2.09814795	H	5.57062	-0.91627	2.78516
C	5.46266000	0.36641000	3.51558000	C	4.50816	0.05938	4.35620
H	4.95267000	1.27642000	3.83558000	H	4.23816	1.10938	4.35620
C	4.47267000	-0.80358000	3.51558000	C	3.27816	-0.82062	4.10620
H	4.93267000	-1.70359000	3.11559000	H	3.50816	-1.88062	3.99620
H	4.31267000	-1.17358000	4.53558000	H	2.65816	-0.80062	4.99620
C	3.16267000	-0.48358000	2.85558000	C	2.32816	-0.34062	3.04620
N	2.11267000	0.06642000	3.56558000	N	1.06816	0.10938	3.39620
H	2.06267000	0.17642000	4.56558000	H	0.63816	0.14938	4.30620
C	2.76267000	-0.44358000	1.54558000	C	2.42816	-0.24062	1.68620
H	3.39267000	-0.83358000	0.76558000	H	3.28816	-0.43062	1.06620
C	1.15267000	0.36641000	2.66558000	C	0.45816	0.62938	2.31620
H	0.18267000	0.77642000	2.91558000	H	-0.46184	1.19938	2.26620
N	1.53267000	0.18642000	1.39558000	N	1.25816	0.39938	1.27620
C	6.49267000	-0.08358000	4.54558000	C	5.17816	-0.37062	5.66620
O	7.26750299	-1.04007165	4.28418350	O	6.17198	-1.14215	5.64094
Cu	0.89267000	0.46642000	-0.52442000	Cu	0.91816	0.37938	-0.79380
O	1.70267000	0.10642000	-5.53442000	O	-0.76184	-2.32062	2.32620
H	1.23267000	-0.52358000	-6.07442000	H	-1.39184	-1.83062	1.78620
H	1.01267000	0.60642000	-5.09442000	H	-1.07184	-3.22062	2.29620
O	-1.23733000	-2.45359000	3.60558000	O	-1.31184	-1.31062	4.73620
H	-1.14733000	-2.00358000	4.44558000	H	-0.95184	-1.47062	3.86620
H	-1.73733000	-1.83358000	3.06558000	H	-0.54184	-1.17062	5.28620
O	4.64267000	0.01642000	-5.18442000	O	-1.79184	-4.78062	1.89620
H	4.77267000	-0.48358000	-5.98442000	H	-1.63184	-5.71062	1.75620
H	3.69267000	0.15642000	-5.14442000	H	-1.70184	-4.39062	1.02620
O	3.17267000	-4.02358000	1.09558000	O	-3.13184	4.80938	0.14620
H	2.41267000	-3.51358000	1.37558000	H	-3.38184	5.73938	0.13620
H	2.99267000	-4.91358000	1.37558000	H	-2.17184	4.82938	0.09620
O	-4.17733000	2.75642000	-0.45442000	O	-0.85184	1.85938	-0.60380
H	-3.78734000	2.39642000	0.34558000	H	-0.99184	2.72938	-0.96380
H	-4.85733000	3.34642000	-0.13441000	H	-1.72184	1.52938	-0.39380
O	0.14267000	-4.90358000	-2.47441000	O	-3.69184	2.99938	-1.65380
H	0.24267000	-5.80358000	-2.15442000	H	-3.53184	2.37938	-0.94380
H	-0.45733000	-4.49358000	-1.84442000	H	-3.73184	3.84938	-1.21380
O	-4.70733000	-0.73358000	-1.72441000	O	1.13816	-3.33062	-5.01380
H	-5.17733000	-0.96358000	-2.52442000	H	1.79816	-3.80062	-5.51380
H	-4.45733000	0.18642000	-1.85442000	H	0.30816	-3.69062	-5.31380
O	0.31267000	3.86641000	3.94558000	O	1.47816	-2.95062	0.44620
H	-0.57733000	3.51642000	3.87558000	H	1.62816	-3.82062	0.07620
H	0.41267000	4.46642000	3.20559000	H	1.17816	-3.12062	1.33620
O	-1.07733000	1.97642000	-0.29441000	O	-1.00184	4.29938	-2.07380
H	-1.56733000	1.66642000	0.47558000	H	-1.74184	3.68938	-2.08380
H	-1.66733000	2.59642000	-0.71442000	H	-1.35184	5.10938	-2.44380
O	-4.18733000	1.68642000	-3.87442000	O	-0.64184	3.62938	2.76620
H	-4.81733000	1.99642000	-3.22441000	H	-1.44184	3.62938	3.29620
H	-3.45733000	2.29641000	-3.81442000	H	-0.75184	4.34938	2.14620
O	2.47267000	-3.26358000	-1.26442000	O	-0.57184	5.83938	0.56620
H	1.88267000	-3.81358000	-1.78442000	H	0.37816	5.72938	0.54620

H	2.72267000	-3.82358000	-0.52442000	H	-0.72184	6.72938	0.23620
O	2.66267000	-0.63359000	-1.47441000	O	2.45816	-1.09062	-1.30380
H	3.59267000	-0.45359000	-1.35442000	H	2.23816	-1.86062	-0.78380
H	2.61267000	-1.58358000	-1.56442000	H	2.69816	-1.45062	-2.16380
O	0.49267000	-2.98358000	1.76558000	O	-4.63184	-0.65062	-1.75380
H	-0.00733000	-2.69358000	2.51558000	H	-4.36184	0.06938	-1.18380
H	-0.09733000	-3.57358000	1.29558000	H	-4.50184	-0.31062	-2.64380
O	-2.11733000	4.36641000	-1.68442000	O	3.00816	-1.34062	-4.24380
H	-1.90733000	4.82642000	-0.87442000	H	2.35816	-2.02062	-4.42380
H	-3.02733000	4.10642000	-1.58442000	H	2.67816	-0.56062	-4.69380
O	-2.28734000	3.67642000	3.12558000	H	4.80079	-0.01475	6.60207
H	-2.42733000	4.47642000	2.61559000	H	5.84011	0.79293	2.86068
H	-2.46733000	2.96642000	2.50558000	H	6.82619	1.30427	-3.81935
H	6.92783488	2.18444332	-3.41012299	H	6.50123	0.83657	-0.05563
H	-6.83573213	-0.74779075	1.71756703	H	-7.03114	-1.13555	0.97718
H	6.44455103	1.84517285	-0.59190812				
H	6.55673999	0.41389165	5.49073448				
H	6.81060482	1.26306176	2.31583373				
Frame 13:				Frame 14:			
N	-0.44877000	-1.04754000	-0.21027000	N	0.09246	-1.37299	-0.00120
H	-0.86877000	-1.00754000	0.70974000	H	-0.03754	-1.19299	0.98880
H	-0.06877000	-1.97754000	-0.11026000	H	1.08246	-1.57299	0.05880
C	-1.63877000	-1.52754000	-0.88026000	C	-0.65754	-2.60299	-0.05120
H	-2.46877000	-0.90754000	-0.54026000	H	-1.61754	-2.51299	0.46880
C	-1.52877000	-1.41754000	-2.41026000	C	-0.94754	-3.09299	-1.47120
H	-0.72877000	-2.07754000	-2.73026000	H	-0.04754	-3.07299	-2.09120
H	-2.40877000	-1.86754000	-2.86026000	H	-1.30754	-4.10299	-1.61120
C	-1.32877000	-0.01754000	-2.93026000	C	-1.85754	-2.17299	-2.24120
N	-0.27877000	0.83246000	-2.62027000	N	-1.71754	-0.79299	-2.20120
C	-2.23877000	0.66246000	-3.70026000	C	-2.89754	-2.53299	-3.06120
H	-3.18877000	0.27246000	-4.05026000	H	-3.32754	-3.46299	-3.39120
C	-0.43877000	1.92246000	-3.38026000	C	-2.74754	-0.37299	-2.95120
H	0.23123000	2.76245000	-3.46027000	H	-3.00754	0.65701	-3.13120
N	-1.60877000	1.84246000	-4.04026000	N	-3.42754	-1.35299	-3.55120
H	-1.96877000	2.54246000	-4.67026000	H	-4.17754	-1.27299	-4.22120
C	-1.94877000	-2.94754000	-0.43026000	C	0.07246	-3.68299	0.74880
O	-1.04877000	-3.72754000	-0.12027000	O	1.24246	-3.90299	0.42880
N	-3.23877000	-3.28754000	-0.34026000	N	-0.50754	-4.32299	1.75880
H	-3.96877000	-2.61754000	-0.55026000	H	-1.47754	-4.09299	1.93880
C	-3.77877000	-4.47754000	0.28973000	C	0.05246	-5.28299	2.68880
H	-4.59877000	-4.91754000	-0.27026000	H	-0.64754	-6.09299	2.91880
H	-3.15877000	-5.35754000	0.44974000	H	1.00246	-5.74299	2.42880
C	-4.44877000	-4.14755000	1.61974000	C	0.16246	-4.69299	4.08880
O	-5.28877000	-4.92754000	2.05974000	O	1.24246	-4.90299	4.62880
N	-4.15877000	-3.01754000	2.27974000	N	-0.80754	-3.90299	4.56880
H	-3.47877000	-2.35754000	1.94974000	H	-1.61754	-3.75299	3.97880
C	-4.72877000	-2.69754000	3.56974000	C	-0.74754	-3.06299	5.73880
H	-4.55877000	-3.51754000	4.26974000	H	-0.17754	-3.77299	6.32880
C	-3.68877000	-1.76754000	4.20974000	C	-0.02754	-1.72299	5.53880
H	-4.04877000	-1.53754000	5.20974000	H	0.20246	-1.45299	6.56880
H	-2.73877000	-2.29754000	4.27974000	H	0.93246	-1.86299	5.03880
C	-3.51877000	-0.36754000	3.60974000	C	-0.81754	-0.56299	4.92880
H	-4.46877000	0.15246000	3.48974000	H	-1.86754	-0.51299	5.18880
H	-3.15877000	0.34246000	4.35974000	H	-0.37754	0.39701	5.17880
C	-2.66877000	-0.27754000	2.34974000	C	-0.82754	-0.59299	3.39880
O	-2.80877000	0.71246000	1.60974000	O	-1.90754	-0.23299	2.87880
O	-1.85877000	-1.19754000	2.12973000	O	0.19246	-0.89299	2.73880
C	-6.15877000	-2.16754000	3.57974000	C	-2.08754	-2.99299	6.45880
O	-6.70984106	-1.86441634	4.66969747	O	-2.24876	-2.18629	7.41107
N	5.40123000	1.79246000	-4.26026000	N	1.50246	1.61701	-6.52120
H	5.33073726	0.79551777	-4.29397882	H	2.16473	0.92524	-6.23334
C	4.74123000	2.28246000	-3.07026000	C	0.93246	2.25701	-5.35120
H	4.91123000	3.35245000	-2.99026000	H	0.43246	3.20701	-5.55120
C	3.26123000	1.88246000	-3.16026000	C	-0.04754	1.30701	-4.67120
H	2.98123000	2.20246000	-4.16026000	H	-0.75754	1.01701	-5.43120
H	3.05123000	0.81246000	-3.05026000	H	0.44246	0.42701	-4.25120
C	2.39123000	2.68246000	-2.23026000	C	-0.79754	2.06701	-3.61120

N	1.81123000	2.19245000	-1.07026000	N	-0.60754	1.84701	-2.24120
C	2.17123000	4.03246000	-2.29026000	C	-1.84754	2.93701	-3.71120
H	2.51123000	4.78246000	-2.99026000	H	-2.42754	3.33701	-4.52120
C	1.44123000	3.29246000	-0.41026000	C	-1.44754	2.62701	-1.56120
H	0.93123000	3.28246000	0.53973000	H	-1.52754	2.69701	-0.49120
N	1.59123000	4.44245000	-1.10026000	N	-2.31754	3.17701	-2.43120
H	1.16123000	5.32246000	-0.87027000	H	-3.14754	3.69701	-2.19120
C	5.41123000	1.63246000	-1.87027000	C	2.20246	2.48701	-4.54120
O	4.98619903	0.53215904	-1.43179875	O	2.62996	1.58721	-3.77233
N	6.05123000	1.45246000	1.74974000	N	4.35246	4.16701	-1.83120
H	6.08765074	0.57907631	1.26404975	H	5.30127	4.03712	-2.11910
C	5.51123000	1.51245000	3.08974000	C	4.32246	4.60701	-0.45120
H	4.98123000	2.43246000	3.32974000	H	3.48246	5.26701	-0.22120
C	4.54123000	0.36246000	3.34974000	C	4.05246	3.38701	0.42880
H	4.95123000	-0.63754000	3.22974000	H	4.89246	2.68701	0.39880
H	4.35123000	0.42246000	4.41974000	H	4.08246	3.78701	1.43880
C	3.22123000	0.39246000	2.63974000	C	2.72246	2.70701	0.23880
N	2.08123000	0.94245000	3.19974000	N	1.84246	2.67701	1.29880
H	2.13123000	1.31246000	4.13974000	H	1.94246	3.26701	2.11880
C	2.85123000	0.18246000	1.33974000	C	2.33246	1.71701	-0.63120
H	3.44123000	-0.07754000	0.46973000	H	2.77246	1.33701	-1.55120
C	1.11123000	0.96246000	2.27974000	C	0.91246	1.74701	1.03880
H	0.16123000	1.36246000	2.60974000	H	0.03246	1.55701	1.62880
N	1.52123000	0.50246000	1.09974000	N	1.16246	1.14701	-0.13120
C	6.59123000	1.38246000	4.15974000	C	5.62246	5.26701	-0.00120
O	7.61024292	0.67670899	3.94271757	O	6.66262	5.14898	-0.69956
Cu	0.60123000	0.53246000	-0.76026000	Cu	-0.25754	0.13701	-1.17120
O	-0.84877000	4.10245000	2.56974000	O	2.58246	-1.46299	2.38880
H	-1.13877000	4.99246000	2.40974000	H	2.90246	-2.08299	3.03880
H	-1.64877000	3.61246000	2.75974000	H	1.65246	-1.36299	2.57880
O	-1.90877000	4.14246000	-1.43026000	O	-4.24754	3.15701	0.55880
H	-1.66877000	4.26245000	-2.35026000	H	-4.88754	2.62701	1.00880
H	-2.11877000	5.02246000	-1.12027000	H	-4.71754	3.53701	-0.18120
O	-3.31877000	2.80246000	3.21973000	O	-4.51754	-0.23299	2.91880
H	-3.19877000	2.06246000	2.62973000	H	-3.56754	-0.09299	2.93880
H	-4.05877000	3.28246000	2.84974000	H	-4.87754	0.50701	3.41880
O	3.58123000	-2.77754000	-0.41026000	O	-2.77754	2.33701	3.50880
H	3.56123000	-3.69754000	-0.66026000	H	-2.56754	1.49701	3.09880
H	3.03123000	-2.71754000	0.36974000	H	-3.55754	2.15701	4.02880
O	-4.94877000	1.80246000	-2.95026000	O	-1.70754	3.79701	1.45880
H	-5.21877000	0.97246000	-3.33026000	H	-2.61754	3.98701	1.24880
H	-4.61877000	1.57246000	-2.08026000	H	-1.74754	3.29701	2.27880
O	-1.01877000	1.97246000	-0.04026000	O	2.57246	-1.28299	-6.42120
H	-1.34877000	2.85245000	-0.24026000	H	2.28246	-1.63299	-7.26120
H	-1.69877000	1.58246000	0.49974000	H	2.23246	-1.89299	-5.77120
O	3.92123000	-0.46754000	-5.46027000	O	3.19246	-2.58299	-1.17120
H	3.89123000	-0.98755000	-6.26026000	H	2.87246	-3.32299	-1.68120
H	3.36123000	-0.93754000	-4.84026000	H	3.06246	-2.83299	-0.26120
O	2.10123000	-4.39755000	-2.82026000	O	1.97246	1.52701	4.25880
H	1.60123000	-5.11754000	-2.43026000	H	1.61246	0.70701	3.89880
H	2.95123000	-4.43754000	-2.39026000	H	1.35246	2.19701	3.98880
O	1.46123000	-2.94754000	1.25974000	O	-4.17754	-1.46299	0.20880
H	1.28123000	-2.46754000	2.06974000	H	-4.58754	-0.78299	0.75880
O	0.78123000	-3.61754000	1.21973000	H	-4.90754	-1.85299	-0.26120
O	1.67123000	-1.77754000	-4.12027000	O	-1.95754	0.34701	0.33880
H	1.61123000	-2.71754000	-3.96027000	H	-1.88754	0.14701	1.27880
H	1.27123000	-1.64755000	-4.98026000	H	-2.81754	0.02701	0.08880
O	-4.37877000	1.63246000	-0.29026000	O	1.52246	-0.76299	-2.38120
H	-4.48877000	2.57246000	-0.10026000	H	2.25246	-1.28299	-2.04120
H	-3.91877000	1.29246000	0.47974000	H	1.45246	-1.04299	-3.30120
O	2.06123000	-0.95754000	-1.50026000	O	1.25246	-2.95299	-4.55120
H	2.75123000	-1.52754000	-1.16026000	H	1.60246	-3.60299	-3.94120
H	1.74123000	-1.41754000	-2.28027000	H	0.41246	-3.31299	-4.82120
O	-0.17877000	-2.39755000	3.95974000	H	5.64968	5.83020	0.90818
H	-0.53877000	-1.97754000	4.73974000	H	3.91984	4.85764	-2.41074
H	-0.66877000	-2.01754000	3.22974000	H	1.96114	2.30291	-7.08613
H	6.24417306	2.11056141	-1.39854456	H	2.73076	3.41361	-4.62618

H	6.36512540	2.05797855	-4.24012135	H	-2.89201	-3.62972	6.15501
H	6.38845851	2.28425467	1.30880393				
H	6.48212925	1.89139456	5.09461038				
H	-6.69348690	-2.05343496	2.65998031				
Frame 15:				Frame 16:			
N	-0.36521	-1.27119	0.30487	N	-1.03239	-1.18098	0.37149
H	0.09479	-1.07119	1.18487	H	-0.53239	-1.36098	1.22149
H	0.35479	-1.95119	0.08487	H	-1.10240	-2.11098	-0.01851
C	-1.42521	-2.02119	0.93487	C	-2.36239	-1.28098	0.94149
H	-1.98521	-1.36119	1.60487	H	-2.56239	-0.41098	1.56149
C	-2.37521	-2.59119	-0.11513	C	-3.35240	-1.30098	-0.21851
H	-1.85521	-3.08119	-0.94513	H	-3.04239	-2.11098	-0.87851
H	-2.96521	-3.37119	0.36487	H	-4.34239	-1.44098	0.21149
C	-3.21521	-1.52119	-0.73513	C	-3.45239	-0.02098	-1.00851
N	-2.72521	-0.28119	-1.16513	N	-2.35240	0.78902	-1.29851
C	-4.56521	-1.51119	-0.97513	C	-4.60240	0.50902	-1.51851
H	-5.28521	-2.26119	-0.67513	H	-5.63239	0.17902	-1.45851
C	-3.77521	0.46881	-1.49513	C	-2.85240	1.88902	-1.86851
H	-3.73521	1.50881	-1.80513	H	-2.34239	2.82902	-2.03851
N	-4.91521	-0.23119	-1.36513	N	-4.18239	1.74902	-1.95851
H	-5.88521	-0.03119	-1.54513	H	-4.75239	2.53902	-2.19851
C	-0.68521	-3.11119	1.68487	C	-2.45239	-2.54098	1.79149
O	0.04479	-3.94119	1.14487	O	-2.12239	-3.60098	1.26149
N	-1.05521	-3.07119	2.97487	N	-2.84239	-2.49098	3.07149
H	-1.80521	-2.50119	3.33487	H	-2.89239	-1.57098	3.47149
C	-0.52521	-3.92119	4.02487	C	-2.86239	-3.60098	4.00149
H	-1.35521	-4.58119	4.25487	H	-3.90239	-3.76098	4.28149
H	0.23479	-4.55119	3.55487	H	-2.46239	-4.53098	3.57149
C	0.10479	-3.08119	5.12487	C	-2.02239	-3.26098	5.22149
O	0.36479	-3.68119	6.17487	O	-2.39239	-3.63098	6.33149
N	0.47479	-1.82119	4.90487	N	-0.95239	-2.49098	5.03149
H	0.21479	-1.37119	4.03487	H	-0.75239	-2.15098	4.10149
C	1.43479	-1.05119	5.66487	C	-0.00239	-2.22098	6.10149
H	2.01479	-1.80119	6.20487	H	0.18761	-3.11098	6.68149
C	2.44479	-0.28119	4.81487	C	1.25761	-1.90098	5.29149
H	3.24479	0.11881	5.43487	H	1.99761	-2.04098	6.08149
H	2.94479	-0.94119	4.10487	H	1.50761	-2.66098	4.55149
C	1.91479	0.96881	4.10487	C	1.44761	-0.47098	4.78149
H	1.50479	1.74881	4.73487	H	1.17761	0.28902	5.52149
H	2.81479	1.40881	3.67487	H	2.48760	-0.22098	4.57149
C	0.83479	0.71881	3.06487	C	0.69761	-0.23098	3.48149
O	0.01479	1.62881	2.80487	O	0.18761	0.90902	3.36149
O	0.93479	-0.33119	2.38487	O	0.38761	-1.16098	2.71149
C	0.87479	-0.08119	6.70487	C	-0.40239	-1.14098	7.09149
O	1.65234	0.67503	7.34293	O	0.34152	-0.87970	8.07225
N	-0.84521	-1.08119	-6.58513	N	0.28761	0.84902	-6.74851
H	-1.29682	-1.80739	-6.06680	H	-0.27626	0.07240	-6.46758
C	-0.66521	0.07881	-5.73513	C	0.85761	1.47902	-5.57851
H	-0.90521	1.01881	-6.22513	H	1.06761	2.53902	-5.74851
C	-1.50521	-0.13119	-4.46513	C	-0.13239	1.36902	-4.41851
H	-2.52521	-0.45119	-4.71513	H	-1.15239	1.56902	-4.74851
H	-1.11521	-0.83119	-3.73513	H	-0.18239	0.38902	-3.96851
C	-1.62521	1.15881	-3.69513	C	0.10761	2.35902	-3.30851
N	-0.96521	1.38881	-2.49513	N	0.17761	1.95902	-1.97851
C	-2.26521	2.28881	-4.12513	C	0.30761	3.70902	-3.35851
H	-2.75521	2.49881	-5.06513	H	0.19761	4.37902	-4.19851
C	-1.18521	2.67881	-2.21513	C	0.37761	3.05902	-1.24851
H	-0.67521	3.28881	-1.48513	H	0.66761	3.07902	-0.20851
N	-1.95521	3.22881	-3.17513	N	0.45761	4.12902	-2.04851
H	-2.12521	4.21881	-3.32513	H	0.48760	5.10902	-1.79851
C	0.81479	0.15881	-5.42513	C	2.06761	0.61902	-5.24851
O	1.33460	-0.65904	-4.62234	O	1.91032	-0.51181	-4.71931
N	4.11479	1.63881	-4.21513	N	5.02761	-0.10098	-3.13851
H	4.71709	0.84068	-4.22967	H	5.14171	-1.03397	-3.47983
C	4.54479	2.54881	-3.17513	C	5.62761	0.00902	-1.81851
H	3.86479	3.38881	-3.01513	H	5.54761	1.00902	-1.39851
C	4.61479	1.77881	-1.85513	C	4.96761	-1.10098	-1.00851

H	5.22479	0.88881	-2.01513	H	4.86761	-2.06098	-1.51851
H	5.11479	2.36881	-1.09513	H	5.52761	-1.24098	-0.07851
C	3.25479	1.43881	-1.30513	C	3.58761	-0.72098	-0.53851
N	2.67479	2.27881	-0.37513	N	3.52761	0.07902	0.59149
H	3.01479	3.13881	0.03487	H	4.27761	0.49902	1.13149
C	2.35479	0.44881	-1.58513	C	2.31761	-0.84098	-1.00851
H	2.48479	-0.41119	-2.21513	H	1.91761	-1.25098	-1.93851
C	1.45479	1.76881	-0.14513	C	2.23760	0.37902	0.79149
H	0.71479	2.28881	0.43487	H	1.79761	0.96902	1.58149
N	1.16479	0.69881	-0.88513	N	1.46761	-0.13098	-0.17851
C	5.90479	3.05881	-3.63513	C	7.08761	-0.41098	-1.90851
O	6.67911	2.29873	-4.27252	O	7.40787	-1.43755	-2.56208
Cu	-0.74521	0.01881	-1.10513	Cu	-0.43239	0.27902	-0.76851
O	0.05479	4.19881	2.59487	O	0.88761	-3.28098	-3.08851
H	-0.52521	4.49881	3.29487	H	1.35761	-3.52098	-2.29851
H	0.09479	3.24881	2.71487	H	1.57760	-3.12098	-3.73851
O	-2.07521	2.30881	4.13487	O	-1.30239	-1.37098	-6.17851
H	-1.18521	2.28881	3.77487	H	-1.79239	-0.97098	-5.45851
H	-2.14521	3.16881	4.55487	H	-1.96239	-1.59098	-6.82851
O	3.77479	-2.75119	-0.45513	O	-3.14239	-1.44098	-4.20851
H	3.49479	-3.66119	-0.41513	H	-4.09239	-1.36098	-4.17851
H	3.33479	-2.33119	0.28487	H	-2.97239	-2.36098	-3.99851
O	2.49479	-2.21119	1.99487	O	-1.73239	4.11902	1.05149
H	2.44479	-2.72119	2.80487	H	-1.13239	4.81902	0.77149
H	1.90479	-1.46119	2.14487	H	-2.05239	4.39902	1.90149
O	-1.42521	1.29881	0.63487	O	2.00761	4.19902	1.74149
H	-1.03521	1.39881	1.50487	H	1.59761	5.00902	1.45149
H	-2.24521	1.78881	0.68487	H	1.72761	4.10902	2.65149
O	-0.72521	-3.41119	-4.94513	O	-0.70239	1.64902	1.01149
H	-1.57521	-3.83119	-4.79513	H	-0.34239	1.35902	1.85149
H	-0.16521	-3.76119	-4.24513	H	-1.13239	2.47902	1.22149
O	-3.84521	2.36881	0.71487	O	2.63761	-4.09098	-0.67851
H	-4.44521	2.55881	-0.00513	H	2.87761	-4.97098	-0.39851
H	-3.84521	3.16881	1.24487	H	2.28761	-3.68098	0.11149
O	0.14479	4.88881	0.13487	O	1.15761	3.19902	4.08149
H	-0.80521	4.95881	0.02487	H	0.48760	3.64902	4.59149
H	0.25479	4.57881	1.02487	H	0.77761	2.33902	3.89149
O	-3.34521	-1.41119	3.95487	O	-0.76240	-1.25098	-2.51851
H	-3.47521	-0.66119	3.37487	H	-1.51240	-1.20098	-3.10851
H	-4.11521	-1.95119	3.83487	H	-0.21239	-1.95098	-2.87851
O	0.59479	-1.92119	-2.21513	O	-2.36239	0.46902	3.84149
H	0.93479	-1.61119	-3.05513	H	-1.44239	0.69902	3.73149
H	1.07479	-2.73119	-2.04513	H	-2.81239	1.30902	3.94149
O	-4.10521	1.00881	2.95487	O	-4.56239	1.26902	1.83149
H	-3.38521	1.61881	3.10487	H	-3.82239	1.85902	1.99149
H	-4.33521	1.13881	2.03487	H	-5.00239	1.62902	1.06149
O	1.12479	-4.61119	-1.85513	O	-3.17240	5.22902	-2.04851
H	1.71479	-4.83119	-1.14513	H	-3.03239	6.16902	-2.18851
H	0.26479	-4.91119	-1.56513	H	-3.15239	5.12902	-1.09851
H	6.20151	4.06327	-3.41622	O	0.96761	-3.46098	1.62149
H	4.15387	2.10206	-5.10050	H	0.79761	-4.21098	2.19149
H	-0.17839	-0.04513	6.89040	H	0.73760	-2.70098	2.15149
H	1.41862	0.91075	-5.88869	H	7.84179	0.16660	-1.41607
H	-1.40963	-0.83314	-7.37247	H	5.47535	0.53937	-3.76260
				H	3.05271	0.97544	-5.46629
				H	1.02266	0.52843	-7.34594
				H	-1.31675	-0.60224	6.95506
Frame 17:				Frame 18:			
N	-0.37949	-1.42958	0.14720	N	-1.42889	-0.23340	-0.01660
H	-0.01949	-1.04958	1.01720	H	-1.54889	-0.33340	0.98340
H	0.33051	-2.13958	0.09720	H	-1.67889	-1.20340	-0.14661
C	-1.61949	-1.88958	0.73720	C	-2.65889	0.46660	-0.30661
H	-2.17949	-1.03958	1.12720	H	-2.45889	1.39660	0.22339
C	-2.62949	-2.36958	-0.30280	C	-2.92889	0.91660	-1.74660
H	-2.11949	-2.97958	-1.03280	H	-2.94889	-0.02340	-2.30661
H	-3.38949	-2.98958	0.17720	H	-3.94889	1.29660	-1.72660
C	-3.20949	-1.29958	-1.19280	C	-1.94889	1.96660	-2.20660

N	-2.44949	-0.29958	-1.80280	N	-0.58889	1.64660	-2.24660
C	-4.54949	-1.08958	-1.37280	C	-2.19889	3.19660	-2.74660
H	-5.35949	-1.62958	-0.90280	H	-3.11889	3.70660	-3.01660
C	-3.36949	0.38042	-2.49280	C	-0.04889	2.75660	-2.75661
H	-3.25949	1.25042	-3.12280	H	0.97111	3.06660	-2.89661
N	-4.61949	-0.02958	-2.25280	N	-0.95889	3.67660	-3.11660
H	-5.43949	0.42042	-2.64280	H	-0.84889	4.57660	-3.55661
C	-1.38949	-3.01958	1.72721	C	-3.89889	-0.26340	0.18340
O	-0.91949	-4.06958	1.29720	O	-4.25889	-1.37340	-0.19660
N	-1.63949	-2.71958	3.00720	N	-4.54889	0.35660	1.17339
H	-2.13949	-1.88958	3.29720	H	-4.24889	1.20660	1.63340
C	-1.31949	-3.73958	3.98720	C	-5.69889	-0.28340	1.78340
H	-2.22949	-3.82958	4.58720	H	-6.55889	0.30660	1.47339
H	-1.13949	-4.73958	3.59720	H	-5.86889	-1.29340	1.40339
C	-0.22949	-3.27958	4.94720	C	-5.48889	-0.30340	3.29340
O	0.69051	-4.07958	5.14720	O	-6.55889	-0.33340	3.90339
N	-0.41949	-2.07958	5.49720	N	-4.28889	-0.19340	3.86340
H	-1.33949	-1.68958	5.33720	H	-3.61889	-0.42340	3.14340
C	0.52051	-1.37958	6.33720	C	-3.81889	-0.06340	5.23340
H	1.01051	-2.20958	6.84720	H	-4.12889	-1.01340	5.65339
C	1.61051	-0.59958	5.60720	C	-2.30889	-0.06340	5.47339
H	2.31051	-0.17958	6.32720	H	-2.23889	-0.05340	6.55340
H	2.23051	-1.33958	5.10720	H	-1.91889	-1.06340	5.28340
C	1.14051	0.39042	4.53720	C	-1.45889	0.99660	4.78340
H	0.50051	1.18042	4.91720	H	-1.93889	1.97660	4.81339
H	2.05051	0.87042	4.17720	H	-0.47889	1.03660	5.25340
C	0.74051	-0.11958	3.15720	C	-1.06889	0.70660	3.34340
O	1.12051	-1.24958	2.76720	O	-1.55889	-0.27340	2.74339
O	-0.12949	0.55042	2.54720	O	-0.29889	1.56660	2.85339
C	-0.19949	-0.62958	7.44720	C	-4.39889	1.14660	5.95340
O	0.45204	0.09981	8.23908	O	-4.42048	1.17967	7.21118
N	-0.92949	0.33042	-7.42280	N	3.13111	-1.01340	-6.21660
H	-0.54511	-0.58830	-7.51339	H	2.62260	-1.87444	-6.22064
C	-0.33949	0.99042	-6.27279	C	3.53111	-0.69340	-4.85660
H	-0.21949	2.06042	-6.43279	H	4.38111	-0.02340	-4.85660
C	-1.06949	0.72042	-4.96280	C	2.31111	-0.05340	-4.18661
H	-2.13949	0.63042	-5.11279	H	1.86111	0.66660	-4.85660
H	-0.81949	-0.25958	-4.56280	H	1.54111	-0.79340	-3.97660
C	-0.86949	1.76042	-3.89280	C	2.73111	0.72660	-2.96660
N	-0.52949	1.52042	-2.56280	N	2.11111	0.63660	-1.71660
C	-1.03949	3.11042	-4.03280	C	3.69111	1.69660	-2.96660
H	-1.36949	3.75042	-4.83280	H	4.27111	2.18660	-3.73661
C	-0.30949	2.69042	-1.97280	C	2.85111	1.48660	-1.00661
H	-0.16949	3.05042	-0.96280	H	2.61111	1.70660	0.03340
N	-0.54949	3.67042	-2.86279	N	3.82111	2.13660	-1.66661
H	-0.69949	4.65042	-2.69280	H	4.40111	2.88660	-1.30661
C	1.03051	0.34042	-6.12280	C	4.03111	-1.93340	-4.13660
O	1.12169	-0.90299	-5.95197	O	3.22097	-2.67158	-3.51827
N	4.69051	0.59042	-4.25280	N	5.02111	-3.87340	-1.45660
H	4.50494	-0.37117	-4.45506	H	4.64275	-4.73569	-1.79319
C	5.41051	0.95042	-3.05280	C	4.92111	-3.83340	-0.01660
H	5.12051	1.94042	-2.69280	H	5.31111	-2.86340	0.30340
C	5.04051	-0.09958	-2.00280	C	3.47111	-3.95340	0.44339
H	5.13051	-1.10958	-2.39280	H	2.90111	-4.70340	-0.11660
H	5.70051	-0.00958	-1.14280	H	3.58111	-4.39340	1.44339
C	3.68051	0.17042	-1.42280	C	2.76111	-2.62340	0.46340
N	3.51051	0.82042	-0.21280	N	2.90111	-1.77340	1.53340
H	4.28051	1.17042	0.32720	H	3.31111	-2.15340	2.37340
C	2.41051	-0.13958	-1.81280	C	1.83111	-2.03340	-0.34661
H	2.01051	-0.65958	-2.67280	H	1.52111	-2.35340	-1.32661
C	2.19051	0.88042	0.06721	C	1.85111	-0.93340	1.55340
H	1.86051	1.52042	0.87720	H	1.52111	-0.35340	2.40339
N	1.46051	0.36042	-0.92280	N	1.20111	-1.03340	0.39340
C	6.88051	0.99042	-3.47280	C	5.72111	-4.94340	0.64340
O	7.27329	0.30769	-4.45421	O	5.76529	-6.08560	0.11709
Cu	-0.49949	-0.06958	-1.23280	Cu	0.28111	0.23660	-0.92660
O	1.57051	3.35042	3.13721	O	2.62111	5.44660	-2.12660

H	0.81051	3.69042	3.60720	H	1.92111	5.15660	-1.54660
H	1.21051	2.75042	2.47721	H	3.42111	5.12660	-1.70660
O	-1.15949	4.90042	0.43720	O	-1.64889	3.83660	2.48340
H	-1.43949	5.79042	0.67720	H	-1.31889	3.06660	2.94339
H	-1.97949	4.45042	0.22721	H	-1.11889	3.87660	1.68340
O	1.86051	-3.12958	0.84720	O	-0.08889	-4.09340	-3.68661
H	1.18051	-3.77958	1.02720	H	-0.89889	-4.44340	-4.05661
H	1.76051	-2.47958	1.53720	H	0.21111	-4.76340	-3.07661
O	-3.75949	1.99042	1.23720	O	3.77111	2.02660	2.59340
H	-3.73949	2.91042	0.95720	H	4.00111	2.95660	2.59340
H	-3.48949	2.01042	2.15720	H	3.07111	1.94660	3.23340
O	1.54051	-3.90958	-2.33280	O	-3.17889	-2.58340	-3.13660
H	2.04051	-3.72958	-1.53280	H	-2.73889	-2.29340	-2.33660
H	1.30051	-4.82958	-2.25280	H	-4.08889	-2.31340	-3.02661
O	1.64051	4.14042	0.50720	O	-4.09889	2.88660	1.91340
H	1.86051	4.26042	1.42720	H	-3.22889	3.27660	2.04340
H	0.69051	4.25042	0.47721	H	-4.29889	3.06660	0.99339
O	2.73051	-3.17958	3.85720	O	-1.00889	-0.33340	-4.71660
H	2.14051	-3.51958	4.52720	H	-1.79889	0.18660	-4.87660
H	2.25051	-2.43958	3.47721	H	-1.03889	-1.02340	-5.38660
O	-1.31949	1.13042	0.46720	O	0.08111	2.14660	0.31339
H	-0.80949	1.01042	1.26720	H	-0.09889	1.89660	1.22339
H	-2.19949	1.37042	0.77720	H	0.38111	3.05660	0.37340
O	-2.91949	-0.64958	4.70720	O	0.89111	4.74660	-0.06660
H	-2.82949	0.20042	4.28720	H	0.32111	5.49660	-0.20660
H	-3.63949	-1.07958	4.24720	H	1.63111	5.09660	0.43340
O	-0.14949	-1.87958	-2.72280	O	-0.49889	-1.48340	-2.41661
H	0.42051	-2.63958	-2.64280	H	-0.15889	-2.35340	-2.62660
H	-0.88949	-2.18958	-3.25280	H	-0.68889	-1.09340	-3.27661
O	-2.11949	1.95042	3.49720	O	-1.36889	-2.80340	2.99339
H	-1.35949	1.42042	3.24720	H	-1.33889	-1.85340	3.00340
H	-1.73949	2.77042	3.82720	H	-1.96889	-3.03340	3.70340
O	-3.71949	4.49042	-0.00280	O	-1.27889	-3.28340	0.28340
H	-4.12949	4.59042	-0.86279	H	-2.15889	-3.57340	0.06339
H	-3.52949	5.39042	0.27720	H	-1.30889	-3.14340	1.23340
O	-2.35949	-3.29958	-4.18279	O	1.80111	1.79660	4.44339
H	-3.08949	-2.96958	-4.70280	H	1.06111	1.58660	3.86340
H	-2.74949	-3.92958	-3.58280	H	1.56111	2.63660	4.83339
H	7.57501	1.59893	-2.93217	H	6.24704	-4.75404	1.55578
H	4.37782	1.30287	-4.88100	H	5.98154	-3.80305	-1.72612
H	-1.26004	-0.72211	7.55482	H	5.07227	-2.17946	-4.15504
H	-0.73016	0.85806	-8.24854	H	3.94481	-1.10413	-6.79077
H	1.91499	0.94125	-6.16272	H	-4.78807	1.96870	5.38984
Frame 19:				Frame 20:			
N	-1.13866	0.63806	0.26522	N	-1.51383	0.14801	-0.09380
H	-1.14867	0.47806	1.26522	H	-1.35383	-0.35199	0.76620
H	-1.73867	-0.14194	0.03522	H	-1.96383	-0.59199	-0.61380
C	-2.10866	1.68806	0.08522	C	-2.75382	0.82801	0.19620
H	-1.73867	2.61806	0.52522	H	-2.51383	1.58801	0.94620
C	-2.34866	2.03806	-1.38478	C	-3.19383	1.59801	-1.04380
H	-2.54866	1.07806	-1.87478	H	-3.23382	1.02801	-1.97380
H	-3.32867	2.48806	-1.50478	H	-4.17383	2.05801	-0.88380
C	-1.16866	2.72806	-2.01478	C	-2.29382	2.76801	-1.35380
N	0.17133	2.37806	-1.83478	N	-0.93382	2.58801	-1.58380
C	-1.30866	3.74806	-2.91478	C	-2.68382	4.07801	-1.35380
H	-2.10866	4.29806	-3.38478	H	-3.66382	4.53801	-1.24380
C	0.79134	3.40806	-2.40478	C	-0.47382	3.83801	-1.65380
H	1.84134	3.65806	-2.32478	H	0.55617	4.14801	-1.77380
N	-0.01866	4.18806	-3.14478	N	-1.49383	4.71801	-1.64380
H	0.14134	5.01806	-3.70478	H	-1.38382	5.68801	-1.88380
C	-3.38866	1.24806	0.77522	C	-3.78383	-0.23199	0.56620
O	-3.97866	0.20806	0.47522	O	-3.86382	-1.25199	-0.10380
N	-3.80866	2.05806	1.74522	N	-4.43382	-0.05199	1.72620
H	-3.12866	2.77806	1.94522	H	-4.35383	0.80801	2.23620
C	-5.11866	2.05806	2.36522	C	-5.22382	-1.10199	2.33620
H	-5.56866	3.04806	2.32522	H	-6.18382	-0.63199	2.58620
H	-5.81866	1.40806	1.84522	H	-5.43382	-1.99199	1.74620

C	-5.08866	1.74806	3.85522	C	-4.72382	-1.67199	3.65620
O	-6.13866	1.82806	4.49522	O	-5.54382	-1.91199	4.53620
N	-3.89867	1.43806	4.36522	N	-3.45382	-2.07199	3.72620
H	-3.08866	1.62806	3.78522	H	-2.81382	-1.78199	2.99620
C	-3.60866	0.83806	5.65522	C	-2.84382	-2.71199	4.86620
H	-4.48867	0.37806	6.08522	H	-3.44383	-3.59199	5.12620
C	-2.49866	-0.21194	5.53522	C	-1.44383	-3.19199	4.47620
H	-2.59866	-0.82194	6.43522	H	-1.03383	-3.83199	5.25620
H	-2.79866	-0.91194	4.74522	H	-1.47382	-3.88199	3.63620
C	-1.04866	0.18806	5.28522	C	-0.43382	-2.04199	4.42620
H	-0.83866	1.08806	5.85522	H	-0.27382	-1.70199	5.44620
H	-0.33866	-0.52194	5.72522	H	0.53617	-2.48199	4.19620
C	-0.74866	0.52806	3.83522	C	-0.49383	-1.03199	3.28620
O	-1.42866	0.01806	2.91522	O	-1.21383	-1.26199	2.29620
O	0.27134	1.22806	3.65522	O	0.08618	0.06801	3.43620
C	-3.19866	1.94806	6.60522	C	-2.88382	-1.99199	6.20620
O	-2.48329	1.68665	7.60696	O	-2.40532	-2.54329	7.23122
N	2.71134	-0.29194	-6.18478	N	2.81618	1.14801	-6.39380
H	1.77153	-0.63200	-6.21840	H	1.98704	0.59030	-6.43238
C	3.20134	-0.36194	-4.82478	C	3.29618	1.20801	-5.02380
H	4.26133	-0.14194	-4.75478	H	4.17618	1.83801	-4.95380
C	2.34134	0.61806	-4.03478	C	2.14617	1.67801	-4.12380
H	2.43134	1.55806	-4.58478	H	1.65618	2.47801	-4.67380
H	1.29134	0.36806	-3.87478	H	1.38618	0.89801	-4.02380
C	2.98134	1.08806	-2.75478	C	2.51618	2.16801	-2.75380
N	2.44134	0.77806	-1.51478	N	1.80617	1.88801	-1.59380
C	4.19134	1.70806	-2.60478	C	3.59618	2.96801	-2.47380
H	4.90134	2.01806	-3.36478	H	4.33618	3.37801	-3.14380
C	3.42133	1.10806	-0.66478	C	2.66617	2.29801	-0.66380
H	3.49134	0.86806	0.38522	H	2.56618	2.24801	0.41620
N	4.42133	1.77806	-1.24478	N	3.62617	3.12801	-1.10380
H	5.14134	2.27806	-0.73478	H	4.25617	3.63801	-0.50380
C	2.98134	-1.79194	-4.32478	C	3.60618	-0.26199	-4.74380
O	1.90954	-2.09601	-3.73966	O	2.67889	-1.05113	-4.42606
N	3.37134	-4.42194	-2.04478	N	4.93618	-2.78199	-2.45380
H	2.62218	-4.95073	-2.44372	H	4.12092	-3.08586	-2.94678
C	3.50134	-4.75194	-0.64478	C	5.10618	-3.12199	-1.06380
H	4.24134	-4.12194	-0.15478	H	5.63618	-2.28199	-0.62380
C	2.21134	-4.51194	0.12522	C	3.69618	-3.42199	-0.53380
H	1.38134	-5.03194	-0.35478	H	3.10618	-4.09199	-1.15380
H	2.22134	-4.96194	1.12522	H	3.73617	-4.14199	0.28620
C	1.79134	-3.08194	0.34522	C	2.83618	-2.21199	-0.26380
N	2.04134	-2.49194	1.57522	N	2.77618	-1.61199	0.97620
H	2.44134	-2.94194	2.38522	H	3.29618	-1.83199	1.81620
C	1.26133	-2.10194	-0.44478	C	1.95618	-1.53199	-1.06380
H	1.02134	-2.18194	-1.49478	H	1.87617	-1.80199	-2.10380
C	1.53134	-1.25194	1.52522	C	1.85618	-0.63199	0.88620
H	1.49134	-0.69194	2.44522	H	1.68618	0.00801	1.73620
N	1.10133	-0.94194	0.29522	N	1.29618	-0.55199	-0.32380
C	3.97134	-6.20194	-0.53478	C	5.88618	-4.42199	-0.92380
O	3.68899	-7.02554	-1.44337	O	5.87880	-5.26402	-1.85896
Cu	0.55134	0.74806	-0.71478	Cu	0.06618	1.00801	-0.90380
O	-1.36866	-4.02194	-1.00478	O	-1.48382	-2.83199	0.29620
H	-1.82867	-3.26194	-0.64478	H	-1.31382	-2.29199	1.05620
H	-2.04866	-4.50194	-1.48478	H	-2.38382	-3.14199	0.41620
O	2.37134	1.08806	5.07522	O	3.50617	1.43801	2.48620
H	2.58134	2.01806	5.17522	H	3.03617	2.24801	2.30620
H	1.56134	1.06806	4.56522	H	3.14617	1.12801	3.31620
O	-0.63866	3.61806	4.52522	O	-0.29382	4.49801	1.79620
H	-0.40866	3.64806	5.45522	H	0.20618	5.02801	1.17620
H	-0.42866	2.72806	4.26522	H	-0.11382	4.88801	2.65620
O	2.64134	4.28806	1.11522	O	-0.84382	-3.01199	-3.47380
H	3.17133	4.68806	0.43522	H	-0.61382	-2.77199	-4.37380
H	1.74134	4.56806	0.91522	H	-1.55382	-3.65199	-3.56380
O	1.20134	1.93806	1.11522	O	-0.05382	-4.52199	-1.27380
H	0.92133	1.76806	2.01522	H	-0.46383	-3.98199	-0.60380
H	1.78134	2.69806	1.18522	H	-0.21383	-4.05199	-2.09380

O	-0.14867	0.19806	-6.61478	O	2.37617	0.23801	4.62620
H	-0.93866	0.41806	-6.11478	H	1.52618	0.06801	4.22620
H	-0.22866	0.69806	-7.42478	H	2.18618	0.82801	5.35620
O	3.97134	0.51806	3.14522	O	-1.68382	1.29801	-4.50380
H	3.44134	0.78806	3.89522	H	-2.18382	0.66801	-5.01380
H	4.42133	1.31806	2.86522	H	-2.07382	2.14801	-4.70380
O	-0.55866	-0.50194	-2.31478	O	0.25617	1.95801	1.34620
H	-1.26866	0.01806	-2.68478	H	0.33618	1.53801	2.20620
H	-0.61866	-1.34194	-2.76478	H	0.07617	2.87801	1.54620
O	-2.32867	0.80806	-4.44478	O	0.26618	-1.36199	-5.61380
H	-2.75866	1.43806	-5.02478	H	0.27618	-0.50199	-6.01380
H	-2.79866	-0.01194	-4.59478	H	1.06618	-1.39199	-5.08380
O	-3.18866	-1.89194	-4.32478	O	-2.00382	1.41801	4.28620
H	-2.43866	-2.29194	-3.88478	H	-1.79382	1.62801	5.19620
H	-3.94866	-2.20194	-3.81478	H	-1.22382	0.97801	3.96620
O	-2.45866	-1.92194	0.21522	O	-4.15382	2.40801	2.74620
H	-2.15866	-2.01194	1.12522	H	-3.82382	3.20801	2.32620
H	-3.38866	-1.69194	0.29522	H	-3.44383	2.13801	3.32620
O	-1.98867	-2.55194	2.80522	O	-0.48382	-0.15199	-2.72380
H	-2.72866	-2.74194	3.38522	H	-0.83383	-1.01199	-2.95380
H	-1.82867	-1.61194	2.92522	H	-0.89382	0.45801	-3.33380
O	-0.73867	-2.85194	-3.55478	O	-3.56382	4.65801	1.45620
H	0.02134	-3.04194	-4.10478	H	-2.62383	4.78801	1.58620
H	-0.60866	-3.40194	-2.77478	H	-3.69383	4.85801	0.52620
H	4.54049	-6.51687	0.31480	H	6.44063	-4.61966	-0.03026
H	4.22377	-4.64112	-2.51946	H	5.63346	-2.24219	-2.92540
H	3.29010	-0.85269	-6.77689	H	4.61169	-0.62024	-4.81793
H	3.73889	-2.53295	-4.47280	H	3.51961	0.74017	-6.97590
H	-3.51784	2.95302	6.42333	H	-3.31881	-1.01696	6.27686

Mono-aqua Complex – Model 1

Frame 1:				Frame 2:			
N	0.283960000	-1.386730000	0.051400000	N	0.817300000	-0.586220000	-0.277840000
H	-0.286040000	-1.576730000	-0.758600000	H	0.427300000	-0.766220000	-1.197840000
H	-0.136040000	-1.966730000	0.771400000	H	0.977300000	-1.566220000	-0.057840000
C	1.373960000	-2.256730000	-0.338600000	C	2.177300000	-0.256220000	-0.657840000
H	1.663960000	-1.926730000	-1.338600000	H	2.167300000	0.463780000	-1.477840000
C	2.483960000	-2.056730000	0.691400000	C	3.067300000	0.263780000	0.462160000
H	2.193960000	-2.106730000	1.741400000	H	2.957300000	-0.186220000	1.442160000
H	3.223960000	-2.836730000	0.551400000	H	4.117300000	0.153780000	0.192160000
C	3.233960000	-0.776730000	0.431400000	C	2.757300000	1.733780000	0.592160000
N	2.623960000	0.473270000	0.321400000	N	1.567300000	2.103780000	1.212160000
C	4.583960000	-0.666730000	0.231400000	C	3.507300000	2.783780000	0.132160000
H	5.423960000	-1.346730000	0.261400000	H	4.477300000	2.793790000	-0.347840000
C	3.613960000	1.343270000	0.131400000	C	1.697290000	3.433780000	1.222160000
H	3.453960000	2.393270000	-0.028600000	H	0.977300000	4.153780000	1.582160000
N	4.793960000	0.703270000	0.191400000	N	2.807300000	3.873780000	0.612160000
H	5.673960000	1.153270000	-0.008600000	H	3.017290000	4.863780000	0.532160000
C	0.903960000	-3.706730000	-0.318600000	C	2.767290000	-1.526210000	-1.247840000
O	0.753960000	-4.236730000	0.771400000	O	2.597300000	-2.566220000	-0.617840000
N	0.643960000	-4.426730000	-1.408600000	N	3.247300000	-1.456210000	-2.487840000
H	0.743960000	-3.946730000	-2.288600000	H	3.507300000	-0.536220000	-2.797840000
C	-0.076040000	-5.686730000	-1.428600000	C	3.717300000	-2.616210000	-3.227840000
H	0.653960000	-6.456730000	-1.668600000	H	4.697290000	-2.446220000	-3.677840000
H	-0.516040000	-5.926730000	-0.458600000	H	3.977300000	-3.436220000	-2.547840000
C	-1.176040000	-5.706730000	-2.478600000	C	2.877290000	-3.096220000	-4.387840000
O	-1.976040000	-6.636730000	-2.438600000	O	3.347300000	-3.876220000	-5.217840000
N	-1.326040000	-4.636730000	-3.268600000	N	1.617300000	-2.656220000	-4.477840000
H	-0.776040000	-3.826730000	-3.018600000	H	1.307300000	-2.096220000	-3.707840000
C	-2.256040000	-4.386730000	-4.348600000	C	0.747300000	-2.686220000	-5.637840000

H	-3.246040000	-4.606730000	-3.948600000	H	0.637300000	-3.726220000	-5.957840000
C	-2.276040000	-2.886730000	-4.628600000	C	-0.672700000	-2.256220000	-5.257840000
H	-3.026040000	-2.616730000	-5.368600000	H	-1.292700000	-2.526210000	-6.117840000
H	-2.706040000	-2.366730000	-3.778600000	H	-1.012700000	-2.896220000	-4.437840000
C	-1.016040000	-2.046730000	-4.878600000	C	-0.842700000	-0.776210000	-4.937840000
H	-0.306040000	-2.516730000	-5.558600000	H	-0.392700000	-0.116210000	-5.677840000
H	-1.306040000	-1.106730000	-5.348600000	H	-1.902700000	-0.526210000	-5.027840000
C	-0.206040000	-1.646730000	-3.658600000	C	-0.332700000	-0.306220000	-3.577840000
O	-0.546040000	-2.026730000	-2.518600000	O	-0.412700000	-1.136220000	-2.647840000
O	0.693960000	-0.786730000	-3.768600000	O	0.377300000	0.723790000	-3.527840000
C	-2.106040000	-5.116730000	-5.668600000	C	1.277300000	-2.076220000	-6.927840000
O	-3.095503510	-5.237814430	-6.436630650	O	0.625215280	-2.200387890	-7.996922980
N	2.923960000	3.543270000	4.861400000	N	-0.432700000	2.323780000	6.692160000
H	3.611720000	2.936620000	4.462700000	H	0.459363900	2.016547720	6.360753410
C	1.913960000	3.843270000	3.871400000	C	-1.362700000	2.393780000	5.582160000
H	1.933960000	4.903270000	3.631400000	H	-2.002700000	3.263780000	5.692160000
C	2.293960000	3.103270000	2.591400000	C	-0.622700000	2.303780000	4.242160000
H	3.333960000	3.373270000	2.391400000	H	0.317300000	2.863780000	4.312160000
H	2.183960000	2.023270000	2.651400000	H	-0.262700000	1.283780000	4.082160000
C	1.443960000	3.463270000	1.401400000	C	-1.192700000	2.933780000	3.002160000
N	0.733960000	2.553270000	0.631400000	N	-1.112700000	2.393780000	1.722160000
C	1.353960000	4.703270000	0.831400000	C	-2.022700000	4.023780000	2.992160000
H	1.743960000	5.643270000	1.191400000	H	-2.402700000	4.623780000	3.802160000
C	0.083960000	3.313270000	-0.248600000	C	-1.712700000	3.263780000	0.912160000
H	-0.506040000	3.053270000	-1.108600000	H	-1.802700000	3.203780000	-0.157840000
N	0.363960000	4.623270000	-0.128600000	N	-2.262700000	4.243780000	1.652160000
H	0.163960000	5.293270000	-0.868600000	H	-2.852700000	5.003780000	1.342160000
C	0.623960000	3.333270000	4.511400000	C	-2.112700000	1.073780000	5.722160000
O	0.389570000	2.097710000	4.556260000	O	-1.475772020	-0.010882510	5.759584020
N	-2.836040000	2.903270000	4.321400000	N	-5.032700000	-0.996220000	3.882160000
H	-2.557840000	1.979850000	4.585770000	H	-5.005208350	-1.849183670	4.403405800
C	-4.146040000	2.853270000	3.691400000	C	-5.732700000	-1.216220000	2.632160000
H	-4.246040000	3.563270000	2.871400000	H	-6.072700000	-0.276210000	2.192160000
C	-4.306040000	1.483270000	3.041400000	C	-4.772700000	-2.006220000	1.732160000
H	-4.016040000	0.693270000	3.731400000	H	-4.352700000	-2.856220000	2.262160000
H	-5.326040000	1.213270000	2.771400000	H	-5.372700000	-2.416220000	0.922160000
C	-3.396040000	1.293270000	1.861400000	C	-3.652700000	-1.266220000	1.062160000
N	-3.726040000	1.163270000	0.521400000	N	-3.682700000	-0.936220000	-0.277840000
H	-4.656040000	1.283270000	0.151400000	H	-4.412700000	-1.186220000	-0.937840000
C	-2.086040000	0.923270000	1.961400000	C	-2.412700000	-0.876220000	1.502160000
H	-1.526040000	0.813270000	2.881400000	H	-1.942700000	-2.106210000	2.462160000
C	-2.596040000	0.793270000	-0.098600000	C	-2.592700000	-0.196220000	-0.517840000
H	-2.626040000	0.673270000	-1.168600000	H	-2.282700000	0.193780000	-1.477840000
N	-1.526040000	0.703270000	0.701400000	N	-1.772700000	-0.116210000	0.522160000
C	-5.246040000	3.023270000	4.721400000	C	-6.882700000	-2.176220000	2.922160000
O	-4.986470000	2.895500000	5.946090000	O	-6.677882790	-3.217208910	3.598889310
O	2.693960000	2.383270000	-3.108600000	Cu	-0.042700000	0.903780000	0.742160000
H	2.533960000	1.903270000	-3.918600000	O	2.317300000	-4.106220000	1.602160000
H	3.643960000	2.453270000	-3.048600000	H	3.067300000	-4.676220000	1.742160000
O	3.393960000	-1.296730000	-3.138600000	H	2.387300000	-3.836220000	0.682160000
H	2.453960000	-1.296730000	-3.338600000	O	2.097300000	2.723790000	-4.067840000
H	3.583960000	-2.196730000	-2.888600000	H	1.417300000	2.053780000	-4.017840000
O	-2.486040000	-2.226730000	-0.998600000	H	2.087290000	3.003780000	-4.987840000
H	-1.746040000	-2.136730000	-1.598600000	O	0.877290000	4.533780000	-2.107840000
H	-3.226040000	-1.836730000	-1.468600000	H	1.497300000	4.143780000	-2.717840000
O	0.593960000	0.783270000	-1.718600000	H	0.127300000	4.793790000	-2.647840000
H	1.253960000	1.383270000	-2.058600000	O	-0.262700000	-2.786220000	1.352160000
H	0.463960000	0.143270000	-2.408600000	H	0.397300000	-3.416220000	1.642160000
O	2.013960000	0.773270000	-5.328600000	H	-0.722700000	-3.226220000	0.642160000
H	1.353960000	1.413270000	-5.588600000	O	-0.082700000	2.153780000	-1.257840000
H	1.553960000	0.183270000	-4.728600000	H	0.197300000	3.033780000	-1.497840000
O	-4.426040000	-0.716730000	-2.158600000	H	-0.102700000	1.673780000	-2.087840000
H	-4.736040000	0.193270000	-2.098600000	O	-3.232700000	-1.746220000	-3.127840000
H	-5.216040000	-1.216730000	-2.378600000	H	-3.542700000	-2.246220000	-3.887840000
O	0.563960000	4.173270000	-3.398600000	H	-2.282700000	-1.876220000	-3.137840000
H	1.153960000	3.553270000	-2.958600000	O	-0.402700000	-3.586220000	-1.247840000
H	0.663960000	3.973270000	-4.328600000	H	-0.082700000	-4.136220000	-1.967840000

Cu	0.573960000	0.483270000	0.461400000	H	-0.442700000	-2.706210000	-1.627840000
H	-0.080260000	4.026640000	4.921520000	H	-5.510533420	-0.296373510	4.413093250
H	3.360780000	4.391920000	5.159700000	H	-7.863292130	-1.964282800	2.550109340
H	-2.170540000	3.280310000	3.677230000	H	2.204310870	-1.541855150	-6.925591890
H	-6.242870000	3.251860000	4.406800000	H	-3.180627820	1.069665400	5.788592150
H	-1.158831740	-5.529062190	-5.947308940	H	-0.340428080	3.228845830	7.107300620
Frame 3:				Frame 4:			
N	0.907110000	-0.105880000	-0.239300000	N	1.050880000	-0.275880000	-0.083860000
H	0.727110000	-0.385880000	-1.189300000	H	0.920880000	-0.975880000	-0.793860000
H	1.207100000	-0.905880000	0.300700000	H	1.000880000	-0.905880000	0.706140000
C	2.237110000	0.444120000	-0.359300000	C	2.490880000	-0.095880000	-0.143860000
H	2.407110000	1.194120000	-1.139300000	H	2.840880000	0.054120000	-1.163860000
C	2.767110000	1.134120000	0.900700000	C	3.010880000	1.104120000	0.636140000
H	2.677100000	0.394120000	1.700700000	H	2.670880000	1.174120000	1.666140000
H	3.847110000	1.294120000	0.870700000	H	4.100880000	1.094120000	0.686140000
C	2.097110000	2.464120000	1.150700000	C	2.630880000	2.424120000	0.016140000
N	0.717100000	2.504120000	1.020700000	N	1.320880000	2.674120000	-0.373860000
C	2.547110000	3.754120000	1.190700000	C	3.420880000	3.484120000	-0.353860000
H	3.577100000	4.074120000	1.190700000	H	4.480880000	3.664120000	-0.243860000
C	0.417110000	3.794120000	1.110700000	C	1.400880000	3.824120000	-1.043860000
H	-0.602900000	4.124120000	0.980700000	H	0.610880000	4.264120000	-1.633860000
N	1.477110000	4.624120000	1.130700000	N	2.650880000	4.304120000	-1.143860000
H	1.437110000	5.634120000	1.010700000	H	2.970880000	5.174120000	-1.553860000
C	3.107100000	-0.775880000	-0.599300000	C	3.110880000	-1.415880000	0.296140000
O	3.007110000	-1.735880000	0.150700000	O	2.860880000	-1.835880000	1.426140000
N	3.677100000	-0.845880000	-1.809300000	N	3.910880000	-2.085880000	-0.533860000
H	3.587110000	-0.115880000	-2.489300000	H	4.180880000	-1.695880000	-1.423860000
C	4.487110000	-1.945880000	-2.299300000	C	4.240880000	-3.475880000	-0.273860000
H	5.517110000	-1.595880000	-2.339300000	H	5.320880000	-3.495880000	-0.163860000
H	4.527100000	-2.685880000	-1.499300000	H	3.910880000	-3.915880000	0.666140000
C	3.867110000	-2.605880000	-3.529300000	C	3.710880000	-4.355880000	-1.393860000
O	3.847110000	-3.835880000	-3.559300000	O	3.280880000	-5.495880000	-1.213860000
N	3.417110000	-1.765880000	-4.459300000	N	3.690880000	-3.805880000	-2.613860000
H	3.417110000	-0.775880000	-4.299300000	H	3.990880000	-2.845880000	-2.603860000
C	2.637100000	-2.115880000	-5.639300000	C	3.240880000	-4.435880000	-3.843860000
H	3.067100000	-3.075880000	-5.919300000	H	3.520880000	-5.495880000	-3.823860000
C	1.147100000	-2.315880000	-5.339300000	C	1.720880000	-4.335880000	-3.943860000
H	0.767110000	-2.935880000	-6.139300000	H	1.440880000	-4.965880000	-4.783860000
H	0.997100000	-3.105880000	-4.599300000	H	1.190880000	-4.745880000	-3.083860000
C	0.217100000	-1.195880000	-4.869300000	C	1.180880000	-2.915880000	-4.153860000
H	0.357100000	-0.285880000	-5.449300000	H	1.720880000	-2.445880000	-4.973860000
H	-0.842890000	-1.365880000	-5.019300000	H	0.190880000	-2.985880000	-4.613860000
C	0.287100000	-0.765880000	-3.419300000	C	1.080880000	-2.025880000	-2.923860000
O	0.077100000	-1.645880000	-2.559300000	O	0.540880000	-2.475880000	-1.893860000
O	0.617110000	0.414120000	-3.149300000	O	1.600880000	-0.895880000	-3.023860000
C	2.947110000	-1.225880000	-6.839300000	C	3.930880000	-4.165880000	-5.163860000
O	2.236280820	-1.296424950	-7.875309580	O	3.392966220	-4.531073520	-6.241288890
N	-0.922900000	1.674120000	6.720700000	N	-2.489120000	5.134120000	4.056140000
H	-0.164407710	1.026122790	6.651496920	H	-1.490211030	5.179847580	4.046660290
C	-1.672900000	1.674120000	5.480700000	C	-2.959120000	4.534120000	2.816140000
H	-2.532900000	2.334120000	5.480700000	H	-3.609120000	5.284120000	2.376140000
C	-0.882890000	2.134120000	4.250700000	C	-1.729120000	4.324120000	1.926140000
H	-0.342890000	3.024120000	4.580700000	H	-1.239120000	5.304120000	1.936140000
H	-0.072890000	1.424120000	4.080700000	H	-0.859120000	3.754120000	2.256140000
C	-1.732890000	2.404120000	3.050700000	C	-1.959120000	3.924120000	0.496140000
N	-1.962900000	1.504120000	2.010700000	N	-1.649120000	2.694120000	-0.073860000
C	-2.592890000	3.464120000	2.910700000	C	-2.469120000	4.714120000	-0.493860000
H	-2.892900000	4.294120000	3.540700000	H	-2.909120000	5.704120000	-0.503860000
C	-2.972890000	1.994120000	1.270700000	C	-2.169120000	2.694120000	-1.303860000
H	-3.312890000	1.724120000	0.290700000	H	-2.279120000	1.784120000	-1.873860000
N	-3.252890000	3.234120000	1.720700000	N	-2.549120000	3.944120000	-1.633860000
H	-3.782900000	3.944120000	1.230700000	H	-2.869120000	4.274120000	-2.523860000
C	-2.152890000	0.254120000	5.220700000	C	-3.639120000	3.234120000	3.206140000
O	-1.353467440	-0.608084350	4.772260710	O	-2.954776450	2.191175890	3.372007570
N	-4.762900000	-2.355880000	3.630700000	N	-5.549120000	0.314120000	2.716140000
H	-3.839832560	-2.727915080	3.728354500	H	-5.168153930	0.023183400	3.593762210
C	-5.302900000	-2.735880000	2.340700000	C	-5.849120000	-0.855880000	1.906140000

H	-5.852900000	-1.925880000	1.870700000	H	-6.249120000	-0.445880000	0.976140000
C	-4.212900000	-3.235880000	1.390700000	C	-4.639120000	-1.795880000	1.956140000
H	-3.572890000	-3.975880000	1.870700000	H	-4.269120000	-1.955880000	2.966140000
H	-4.682890000	-3.875880000	0.650700000	H	-4.869120000	-2.825880000	1.676140000
C	-3.312890000	-2.185880000	0.790700000	C	-3.499120000	-1.275880000	1.126140000
N	-3.292890000	-1.935880000	-0.569300000	N	-3.319120000	-1.685880000	-0.173860000
H	-3.912890000	-2.235880000	-1.299300000	H	-3.879120000	-2.355880000	-0.693860000
C	-2.232890000	-1.555880000	1.340700000	C	-2.539120000	-0.325880000	1.356140000
H	-1.982890000	-1.675880000	2.390700000	H	-2.379120000	0.274120000	2.246140000
C	-2.432890000	-0.915880000	-0.719300000	C	-2.299120000	-0.955880000	-0.663860000
H	-2.162890000	-0.505880000	-1.689300000	H	-2.039120000	-1.045880000	-1.703860000
N	-1.672900000	-0.725880000	0.370700000	N	-1.739120000	-0.2145880000	0.236140000
C	-6.292890000	-3.875880000	2.520700000	C	-7.039120000	-1.555880000	2.536140000
O	-6.026949730	-4.821960710	3.306688310	O	-7.041927070	-1.805047060	3.769622250
Cu	-0.482890000	0.834120000	0.760700000	Cu	-0.169120000	1.284120000	-0.043860000
O	1.307110000	-2.745880000	3.310700000	O	-1.769120000	-0.815880000	4.596140000
H	1.967100000	-3.275880000	2.860700000	H	-1.659120000	-1.555880000	3.996140000
H	0.467100000	-3.105880000	3.020700000	H	-2.559120000	-1.025880000	5.096140000
O	1.277100000	2.854120000	-2.969300000	O	-3.509120000	0.824120000	-3.523860000
H	1.007110000	1.954120000	-3.139300000	H	-3.279120000	1.294120000	-4.323860000
H	1.597110000	3.174120000	-3.809300000	H	-3.289120000	-0.085880000	-3.703860000
O	3.537100000	1.014120000	-3.799300000	O	0.890880000	2.814120000	-3.913860000
H	2.637100000	1.304120000	-3.619300000	H	0.720880000	2.334120000	-4.723860000
H	4.077100000	1.724120000	-3.449300000	H	0.590880000	3.704120000	-4.093860000
O	-0.052900000	-4.375880000	1.610700000	O	-1.279120000	-2.895880000	2.976140000
H	0.227110000	-4.285880000	0.700700000	H	-0.879120000	-3.655880000	3.396140000
H	0.337110000	-5.195880000	1.900700000	H	-1.059120000	-2.985880000	2.046140000
O	1.167110000	-3.785880000	-0.819300000	O	-2.729120000	-1.855880000	-3.933860000
H	1.997100000	-3.375880000	-0.579300000	H	-2.969120000	-1.825880000	-4.853860000
H	0.727110000	-3.125880000	-1.349300000	H	-2.599120000	-2.785880000	-3.743860000
O	-4.842890000	1.344120000	-2.339300000	O	3.540880000	0.424120000	-4.613860000
H	-4.272890000	2.104120000	-2.459300000	H	3.510880000	0.344120000	-5.563860000
H	-4.382890000	0.624120000	-2.769300000	H	2.740880000	-0.005880000	-4.303860000
O	-0.912890000	1.614120000	-1.409300000	O	-0.119120000	0.824120000	-2.233860000
H	-0.342890000	1.274120000	-2.099300000	H	0.510880000	0.174120000	-2.543860000
H	-1.062890000	2.524120000	-1.649300000	H	0.060880000	1.604120000	-2.763860000
O	-0.842890000	4.324120000	-2.009300000	O	3.960880000	-1.165880000	3.716140000
H	-0.022890000	4.004120000	-2.369300000	H	3.540880000	-1.565880000	2.966140000
H	-1.482890000	4.204120000	-2.709300000	H	4.280880000	-1.905880000	4.236140000
O	-1.772890000	-3.395880000	-3.099300000	O	-0.079120000	-3.335880000	0.546140000
H	-1.142900000	-4.095880000	-3.289300000	H	0.160880000	-3.215880000	-0.373860000
H	-1.222890000	-2.625880000	-2.959300000	H	0.460880000	-4.065880000	0.846140000
O	-0.972890000	7.004120000	-1.519300000	H	-7.875775320	-1.837570910	1.931525990
H	-1.012900000	6.054120000	-1.569300000	H	-6.388254810	0.834869300	2.873216230
H	-1.682890000	7.304120000	-2.079300000	H	-2.864240710	6.057015050	4.143025990
H	-7.215662900	-3.873649100	1.979049560	H	-4.700304380	3.204618560	3.339995800
H	-4.729140920	-1.358670160	3.697279650	H	4.875993910	-3.664508870	-5.180792230
H	-1.523559260	1.405040720	7.473564390				
H	-3.170224160	-0.011502800	5.419133220				
H	3.768912760	-0.541783850	-6.799895830				
Frame 5:				Frame 6:			
N	0.838200000	-0.464590000	-0.092610000	N	1.066670000	0.219910000	-0.166230000
H	0.458200000	-1.334590000	-0.422610000	H	0.866670000	-0.750090000	-0.366230000
H	1.098200000	-0.774600000	0.827390000	H	1.716670000	0.099910000	0.603770000
C	2.048200000	-0.614600000	-0.872610000	C	2.066670000	0.519910000	-1.166230000
H	1.538200000	-0.954600000	-1.772610000	H	1.786670000	0.129910000	-2.146230000
C	2.748190000	0.745400000	-0.942610000	C	2.186660000	2.039910000	-1.296230000
H	2.918200000	1.005410000	0.107390000	H	2.256670000	2.449910000	-0.286230000
H	3.688200000	0.615410000	-1.472610000	H	3.086670000	2.249910000	-1.866230000
C	1.988200000	1.795400000	-1.692610000	C	0.956670000	2.659910000	-1.906230000
N	0.738200000	2.275410000	-1.312610000	N	-0.323330000	2.519910000	-1.396230000
C	2.348200000	2.435410000	-2.852610000	C	0.946670000	3.419910000	-3.046230000
H	3.238200000	2.245400000	-3.422610000	H	1.726670000	3.679910000	-3.756230000
C	0.398200000	3.165410000	-2.232610000	C	-1.073330000	3.069910000	-2.356230000
H	-0.481800000	3.795400000	-2.232610000	H	-2.143330000	3.199910000	-2.276230000
N	1.278200000	3.205410000	-3.252610000	N	-0.383330000	3.589910000	-3.386230000

H	1.158200000	3.835400000	-4.032610000	H	-0.793330000	4.029910000	-4.196230000
C	2.958200000	-1.754600000	-0.432610000	C	3.386670000	-0.110090000	-0.736230000
O	3.178200000	-1.844600000	0.777390000	O	3.936660000	0.119910000	0.333770000
N	3.608200000	-2.404590000	-1.392610000	N	3.916670000	-1.000090000	-1.586230000
H	3.388200000	-2.214590000	-2.362610000	H	3.486670000	-1.130090000	-2.486230000
C	4.408200000	-3.604590000	-1.262610000	C	4.996670000	-1.940090000	-1.336230000
H	5.278200000	-3.424590000	-1.882610000	H	5.786670000	-1.630090000	-2.016230000
H	4.578200000	-3.804590000	-0.202610000	H	5.456670000	-1.840090000	-0.356230000
C	3.678200000	-4.874590000	-1.682610000	C	4.746670000	-3.430090000	-1.546230000
O	4.338200000	-5.904590000	-1.622610000	O	5.686670000	-4.190090000	-1.776230000
N	2.348200000	-4.824600000	-1.822610000	N	3.476670000	-3.810090000	-1.426230000
H	1.818200000	-3.964590000	-1.892610000	H	2.696670000	-3.200090000	-1.246230000
C	1.528200000	-5.994590000	-2.042610000	C	2.906670000	-5.070090000	-1.856230000
H	1.888200000	-6.884590000	-1.522610000	H	3.386670000	-5.830090000	-1.246230000
C	0.038200000	-5.774600000	-1.782610000	C	1.396670000	-5.160090000	-1.636230000
H	-0.571800000	-6.634590000	-2.072610000	H	1.026660000	-6.180090000	-1.726230000
H	-0.121800000	-5.564590000	-0.722610000	H	1.146670000	-4.930090000	-0.606230000
C	-0.571800000	-4.604590000	-2.562610000	C	0.516670000	-4.220090000	-2.476230000
H	-0.271800000	-4.744590000	-3.602610000	H	0.796670000	-4.250090000	-3.526230000
H	-1.651800000	-4.544590000	-2.542610000	H	-0.503330000	-4.580090000	-2.316230000
C	-0.221800000	-3.184600000	-2.152610000	C	0.506670000	-2.760090000	-2.056230000
O	-0.091800000	-2.294590000	-3.012610000	O	0.326670000	-1.900090000	-2.936230000
O	0.148200000	-2.974590000	-0.972610000	O	0.876670000	-2.420090000	-0.906230000
C	1.648200000	-6.694590000	-3.392610000	C	3.336670000	-5.610090000	-3.216230000
O	0.968937270	-7.727329680	-3.628452030	O	3.382550090	-6.851967580	-3.414234150
N	-0.701800000	6.615410000	2.797390000	N	-2.733330000	5.529910000	3.443770000
H	0.235908410	6.268370640	2.813718860	H	-1.789654850	5.469813230	3.769139920
C	-1.561800000	5.655400000	2.127390000	C	-3.323330000	4.419910000	2.723770000
H	-2.301800000	6.235410000	1.577390000	H	-4.343330000	4.639910000	2.443770000
C	-0.871800000	4.845410000	1.027390000	C	-2.493330000	4.149910000	1.463770000
H	-0.241800000	5.485410000	0.417390000	H	-2.523330000	5.099910000	0.923770000
H	-0.201800000	4.105410000	1.467390000	H	-1.473340000	4.039910000	1.823770000
C	-1.771800000	4.045400000	0.127390000	C	-3.053330000	3.179910000	0.463770000
N	-1.731800000	2.655400000	-0.012610000	N	-2.563340000	1.889910000	0.283770000
C	-2.751800000	4.545400000	-0.692610000	C	-4.203330000	3.249910000	-0.276230000
H	-3.031800000	5.575410000	-0.852610000	H	-4.893330000	4.079910000	-0.396230000
C	-2.691800000	2.385400000	-0.902610000	C	-3.413330000	1.259910000	-0.536230000
H	-3.071800000	1.445410000	-1.272610000	H	-3.373330000	0.229910000	-0.866230000
N	-3.281800000	3.485410000	-1.392610000	N	-4.373330000	2.079910000	-0.986230000
H	-3.961800000	3.485410000	-2.132610000	H	-5.123330000	1.809910000	-1.596230000
C	-2.151800000	4.935410000	3.337390000	C	-3.373330000	3.249910000	3.693770000
O	-1.432670830	4.161990120	4.021674660	O	-2.372088000	2.499227290	3.826285980
N	-4.041800000	1.975400000	4.837390000	N	-4.073330000	-0.140090000	4.953770000
H	-3.133432020	2.070848350	5.244522930	H	-3.481801300	-0.048451450	5.754829410
C	-4.551800000	0.655400000	4.497390000	C	-4.173330000	-1.540090000	4.583770000
H	-5.101800000	0.695410000	3.557390000	H	-4.823330000	-1.680090000	3.713770000
C	-3.331800000	-0.254600000	4.307390000	C	-2.773330000	-2.080090000	4.283770000
H	-2.551800000	0.015400000	5.017390000	H	-2.073330000	-1.810090000	5.063770000
H	-3.551800000	-1.314590000	4.457390000	H	-2.873330000	-3.160090000	4.343770000
C	-2.861800000	-0.274600000	2.877390000	C	-2.133330000	-1.670090000	2.983770000
N	-3.171800000	-1.304590000	2.017390000	N	-2.253330000	-2.430090000	1.833770000
H	-3.791800000	-2.074600000	2.247390000	H	-2.653340000	-3.350090000	1.733770000
C	-1.941800000	0.505410000	2.227390000	C	-1.553330000	-0.500090000	2.583770000
H	-1.461800000	1.375410000	2.647390000	H	-1.323330000	0.359910000	3.193770000
C	-2.581800000	-1.044590000	0.847390000	C	-1.693330000	-1.720090000	0.833770000
H	-2.541800000	-1.584590000	-0.092610000	H	-1.543330000	-2.110090000	-0.166230000
N	-1.791800000	0.025410000	0.927390000	N	-1.253330000	-0.520090000	1.223770000
C	-5.421800000	0.125410000	5.627390000	C	-4.763330000	-2.340090000	5.733770000
O	-5.157012500	0.427318430	6.819996150	O	-4.514275300	-2.010572030	6.922450040
Cu	-0.431800000	1.085400000	-0.122610000	Cu	-0.693330000	1.089910000	-0.006230000
O	-1.741800000	1.725400000	-3.842610000	O	1.376670000	-3.520090000	1.343770000
H	-0.991800000	1.565400000	-4.412610000	H	2.076670000	-2.890090000	1.493770000
H	-2.491800000	1.715410000	-4.422610000	H	1.106670000	-3.360090000	0.433770000
O	0.398200000	-1.654590000	2.647390000	O	2.606670000	-1.960090000	-4.116230000
H	1.328200000	-1.564590000	2.857390000	H	2.676670000	-1.230090000	-4.736230000
H	0.318200000	-2.544590000	2.307390000	H	1.716670000	-1.890090000	-3.766230000
O	3.678200000	-1.574600000	3.527390000	O	-4.333330000	-1.930090000	-1.586230000

H	3.838200000	-1.464590000	2.597390000	H	-3.833330000	-2.740090000	-1.546230000
H	4.238200000	-2.304590000	3.787390000	H	-4.543330000	-1.830090000	-2.516230000
O	-0.221800000	-4.174590000	1.427390000	O	3.786670000	-2.310090000	1.703770000
H	0.218200000	-3.814590000	0.657390000	H	4.576670000	-2.820090000	1.513770000
H	0.338200000	-4.894590000	1.717390000	H	4.066670000	-1.400090000	1.643770000
O	-1.191800000	-0.124590000	-1.892610000	O	-2.513330000	0.759910000	-4.136230000
H	-0.911800000	-0.974590000	-2.242610000	H	-3.253330000	0.139910000	-4.116230000
H	-1.521800000	0.345410000	-2.662610000	H	-1.823330000	0.299910000	-4.606230000
O	1.798200000	0.595410000	-5.372610000	O	-1.113330000	-0.110090000	-1.836230000
H	0.898200000	0.315400000	-5.252610000	H	-0.553330000	-0.770090000	-2.246230000
H	2.268200000	0.235410000	-4.622610000	H	-1.773330000	0.099910000	-2.506230000
O	-0.691800000	-0.904590000	-5.242610000	O	-0.363330000	-0.690090000	-5.286230000
H	-1.641800000	-0.844600000	-5.342610000	H	-0.233330000	-1.300090000	-4.556230000
H	-0.561800000	-1.444590000	-4.462610000	H	0.456670000	-0.720090000	-5.766230000
H	-6.258811620	-0.504037750	5.408056730	H	3.599332910	-4.932985340	-4.002001900
H	2.309941290	-6.307478790	-4.139030380	H	-4.259855040	3.064925090	4.263641860
H	-3.176791940	5.088402750	3.603631890	H	-3.269730690	6.356234990	3.615412980
H	-0.726671200	7.485555950	2.305223920	H	-4.983533980	0.213556120	5.169323080
H	-4.599741480	2.786937900	4.663874740	H	-5.390408720	-3.183408060	5.532556350
Frame 7:				Frame 8:			
N	1.266140000	0.083860000	-0.741400000	N	1.016830000	-0.811000000	0.356670000
H	1.226140000	-0.836140000	-0.311400000	H	0.266830000	-1.391000000	0.686670000
H	2.126140000	0.443860000	-0.351410000	H	1.696830000	-0.961000000	1.086670000
C	1.776140000	-0.486140000	-1.961400000	C	1.636830000	-1.731000000	-0.573330000
H	1.066140000	-1.176140000	-2.411400000	H	0.926830000	-2.211000000	-1.253330000
C	1.946140000	0.633860000	-3.001400000	C	2.786830000	-1.061000000	-1.323330000
H	2.606140000	1.423860000	-2.631400000	H	3.516830000	-0.641000000	-0.633340000
H	2.336140000	0.243860000	-3.941410000	H	3.316840000	-1.791000000	-1.933330000
C	0.626140000	1.153860000	-3.501400000	C	2.236830000	-0.101000000	-2.353330000
N	-0.353860000	1.743860000	-2.711400000	N	1.466830000	1.019000000	-2.073330000
C	0.146140000	1.013860000	-4.771400000	C	2.576830000	0.029000000	-3.673330000
H	0.606140000	0.543860000	-5.631400000	H	3.256830000	-0.601000000	-4.233330000
C	-1.373860000	1.963860000	-3.551400000	C	1.206830000	1.619000000	-3.233330000
H	-2.263860000	2.463860000	-3.201400000	H	0.546830000	2.469000000	-3.383340000
N	-1.133860000	1.543860000	-4.801400000	N	1.936830000	1.109000000	-4.233330000
H	-1.843860000	1.433860000	-5.501400000	H	1.906840000	1.239000000	-5.233330000
C	3.066140000	-1.246140000	-1.681400000	C	2.226840000	-2.781000000	0.346670000
O	4.016140000	-0.706140000	-1.111400000	O	2.856830000	-2.371000000	1.326670000
N	3.166140000	-2.546140000	-1.931400000	N	1.916830000	-4.061000000	0.126670000
H	2.306140000	-3.026140000	-2.181400000	H	1.346830000	-4.241000000	-0.683330000
C	4.226140000	-3.526140000	-1.771400000	C	2.236830000	-5.071000000	1.126670000
H	4.546140000	-3.896140000	-2.751400000	H	2.996830000	-5.801000000	0.856670000
H	5.066140000	-2.996140000	-1.331400000	H	2.556830000	-4.571000000	2.046670000
C	3.866140000	-4.626140000	-0.781410000	C	0.976840000	-5.821000000	1.546670000
O	4.526140000	-5.656140000	-0.911400000	O	1.086830000	-7.001000000	1.866660000
N	2.946140000	-4.396140000	0.158600000	N	-0.183160000	-5.181000000	1.526660000
H	2.476140000	-3.516140000	0.338600000	H	-0.143170000	-4.211000000	1.236670000
C	2.456140000	-5.396140000	1.078600000	C	-1.463170000	-5.751000000	1.916670000
H	3.406140000	-5.676140000	1.548600000	H	-1.263170000	-6.021000000	2.956660000
C	1.476140000	-4.796140000	2.078600000	C	-2.513170000	-4.661000000	2.086670000
H	1.136140000	-5.546140000	2.788600000	H	-3.463170000	-5.071000000	2.436670000
H	1.986140000	-3.996140000	2.628600000	H	-2.353170000	-3.961000000	2.916670000
C	0.166140000	-4.236140000	1.518600000	C	-2.733170000	-3.861000000	0.806670000
H	-0.343860000	-5.106140000	1.098600000	H	-2.433160000	-4.511000000	-0.023330000
H	-0.413860000	-3.826140000	2.338600000	H	-3.813170000	-3.761000000	0.686670000
C	0.356140000	-3.036140000	0.588600000	C	-1.953170000	-2.561000000	0.766670000
O	-0.453860000	-2.846140000	-0.341400000	O	-2.493170000	-1.521000000	0.306670000
O	1.406140000	-2.376140000	0.748600000	O	-0.833170000	-2.471000000	1.296670000
C	1.936140000	-6.726140000	0.548600000	C	-2.073170000	-6.961000000	1.236670000
O	1.703772030	-7.672969670	1.344269070	O	-3.004713940	-7.594748760	1.797168850
N	-0.393860000	6.983860000	-0.451400000	N	3.426830000	6.219000000	-1.413330000
H	0.534864740	6.766660870	-0.751891100	H	4.102492920	5.555883630	-1.091217760
C	-1.263860000	5.933860000	0.018600000	C	2.116830000	5.879000000	-0.873330000
H	-2.313860000	6.233860000	0.078600000	H	1.366830000	6.589000000	-1.213330000
C	-1.213860000	4.783860000	-0.971400000	C	1.626830000	4.539000000	-1.413330000
H	-1.453860000	5.153860000	-1.961400000	H	1.476840000	4.469000000	-2.493330000

H	-0.303860000	4.183860000	-1.121400000	H	2.366830000	3.759000000	-1.223340000
C	-2.253860000	3.703860000	-0.811400000	C	0.196830000	4.169000000	-1.153330000
N	-2.043860000	2.333860000	-0.641400000	N	-0.203170000	2.919000000	-0.703330000
C	-3.593860000	3.963860000	-0.761400000	C	-0.863170000	4.899000000	-1.643330000
H	-4.223860000	4.803860000	-1.001400000	H	-0.863170000	5.869000000	-2.113330000
C	-3.263860000	1.803860000	-0.521400000	C	-1.513170000	2.959000000	-0.923330000
H	-3.413860000	0.743860000	-0.371400000	H	-2.253170000	2.229000000	-0.613330000
N	-4.203860000	2.753860000	-0.481400000	N	-1.973170000	4.139000000	-1.363330000
H	-5.193860000	2.553860000	-0.551400000	H	-2.953170000	4.329000000	-1.523330000
C	-0.833860000	5.493860000	1.408600000	C	2.226840000	5.689000000	0.636670000
O	0.210634030	4.807735170	1.556368370	O	2.721472400	4.630110090	1.103212080
N	-1.213860000	3.453860000	4.768600000	N	0.846830000	5.099000000	3.966670000
H	-0.385262150	3.748549370	5.244608180	H	1.719882350	4.657772990	3.759068650
C	-1.723860000	2.243860000	5.388600000	C	-0.093160000	4.459000000	4.866660000
H	-2.773860000	2.083860000	5.158600000	H	-1.083170000	4.559000000	4.436670000
C	-0.903860000	1.023860000	4.988600000	C	0.296830000	2.979000000	4.856670000
H	0.096140000	1.233860000	5.368600000	H	1.376830000	2.889000000	4.956660000
H	-1.143860000	0.073860000	5.488600000	H	0.036830000	2.499000000	5.806670000
C	-0.893860000	0.683860000	3.528600000	C	-0.183160000	2.239000000	3.646670000
N	-1.493860000	-0.476140000	3.088600000	N	-1.203170000	1.309000000	3.666670000
H	-1.883860000	-1.186140000	3.688600000	H	-1.803170000	1.069000000	4.436670000
C	-0.413860000	1.273860000	2.378600000	C	0.196830000	2.249000000	2.326670000
H	0.116140000	2.203860000	2.268600000	H	0.956830000	2.849000000	1.836670000
C	-1.453860000	-0.466140000	1.738600000	C	-1.333170000	0.779000000	2.446670000
H	-1.853860000	-1.216140000	1.068600000	H	-1.973170000	-0.061000000	2.216670000
N	-0.803860000	0.583860000	1.238600000	N	-0.433160000	1.259000000	1.576670000
C	-1.563860000	2.413860000	6.898590000	C	0.036830000	5.039000000	6.266670000
O	-0.724165930	3.233021510	7.354066520	O	1.137699760	5.511046170	6.652453280
Cu	-0.433860000	1.183860000	-0.681400000	Cu	0.576830000	1.089000000	-0.193330000
O	5.816140000	0.253860000	0.868600000	O	0.076830000	-1.911000000	3.926670000
H	6.096140000	-0.336140000	1.568600000	H	0.716830000	-2.571000000	4.196670000
H	5.156140000	-0.246140000	0.398590000	H	-0.173170000	-2.171000000	3.046670000
O	-4.203860000	1.013860000	-4.221400000	O	-0.373170000	-4.331000000	-1.853330000
H	-4.893860000	0.803860000	-3.591400000	H	-1.223170000	-4.121000000	-2.223340000
H	-3.703860000	0.203860000	-4.311400000	H	0.256830000	-3.991000000	-2.493330000
O	-3.093860000	-3.356140000	0.098600000	O	-4.103170000	1.919000000	1.066670000
H	-3.223860000	-3.756140000	0.958600000	H	-4.353170000	1.009000000	1.236670000
H	-2.153860000	-3.176140000	0.058590000	H	-4.663170000	2.179000000	0.326670000
O	3.016140000	0.393860000	3.708600000	O	-5.103170000	2.119000000	-1.443330000
H	3.806140000	0.513860000	4.248600000	H	-4.303170000	1.909000000	-1.913330000
H	3.266140000	-0.246140000	3.048600000	H	-5.813170000	1.729000000	-1.953330000
O	-5.983860000	0.363860000	-2.441410000	O	1.616830000	-3.431000000	-3.613330000
H	-6.923860000	0.533860000	-2.361400000	H	2.016830000	-3.981000000	-4.273330000
H	-5.743860000	-0.046140000	-1.611400000	H	1.366830000	-2.631000000	-4.093330000
O	-4.993860000	-1.096140000	1.188600000	O	-1.253170000	-0.041000000	-1.473340000
H	-5.823860000	-1.366140000	0.788600000	H	-1.833170000	-0.651000000	-1.033330000
H	-4.403860000	-1.826140000	0.998600000	H	-0.883170000	-0.541000000	-2.203330000
O	3.686140000	-1.496140000	1.858600000	O	5.496830000	-2.771000000	1.866660000
H	4.246140000	-2.266140000	1.848600000	H	4.576830000	-2.531000000	1.766670000
H	2.816140000	-1.836140000	1.648590000	H	5.786830000	-2.971000000	0.976670000
O	-1.453860000	-0.666140000	-1.341400000	O	-4.023160000	-2.501000000	-1.743330000
H	-1.013860000	-1.486140000	-1.091400000	H	-4.943170000	-2.241000000	-1.673330000
H	-2.143860000	-0.946140000	-1.951400000	H	-3.593160000	-2.031000000	-1.033330000
O	3.316140000	1.433860000	1.058590000	O	-0.573170000	-1.381000000	-3.953330000
H	3.176140000	1.023860000	1.918600000	H	-1.193170000	-2.111000000	-3.933330000
H	4.226140000	1.243860000	0.848600000	H	-0.853170000	-0.851000000	-4.703330000
O	0.816140000	-3.866140000	-2.561400000	O	-3.483170000	1.499000000	-3.543340000
H	0.126140000	-3.976140000	-3.211400000	H	-4.123170000	0.919000000	-3.953330000
H	0.356140000	-3.666140000	-1.741400000	H	-3.633170000	2.349000000	-3.953330000
O	-3.213860000	-1.626140000	-2.911400000	O	-4.893170000	-0.571000000	1.226670000
H	-2.753860000	-2.196140000	-3.541400000	H	-5.433160000	-0.371000000	0.456660000
H	-4.053860000	-2.066140000	-2.761400000	H	-4.113170000	-0.981000000	0.876670000
H	-2.165793150	1.836388340	7.568741450	O	-1.243170000	1.169000000	-5.223340000
H	-1.905022280	4.174321990	4.825426240	H	-1.873170000	1.169000000	-4.513330000
H	-1.419294470	5.767538950	2.261399110	H	-1.413170000	1.989000000	-5.693330000
H	-0.719391770	7.929050640	-0.476771760	H	-1.711599840	-7.276092090	0.280174320
H	1.768440500	-6.855334570	-0.500249680	H	1.883403910	6.456124540	1.298841880

				H	3.686233200	7.134854700	-1.106866050
				H	0.621944390	5.981536720	3.553686460
				H	-0.807775990	5.045656950	6.923553860
Frame 9:				Frame 10:			
N	-0.266190000	-1.147620000	0.573490000	N	-0.189650000	-0.660350000	-1.228680000
H	-0.896190000	-0.717620000	1.233490000	H	-0.699650000	-1.270350000	-0.598690000
H	0.433810000	-1.517620000	1.193490000	H	0.290350000	-1.370350000	-1.768680000
C	-1.036190000	-2.327620000	0.243490000	C	-1.259650000	-0.370350000	-2.158680000
H	-2.096190000	-2.227620000	0.013490000	H	-2.069650000	0.269650000	-1.798680000
C	-0.376190000	-3.017620000	-0.956510000	C	-0.659650000	0.469650000	-3.278690000
H	0.623810000	-3.417620000	-0.756510000	H	0.290350000	-0.010350000	-3.518680000
H	-0.946190000	-3.887620000	-1.246510000	H	-1.229650000	0.429650000	-4.208680000
C	-0.406190000	-2.247620000	-2.246510000	C	-0.239650000	1.859650000	-2.878680000
N	0.133810000	-0.977620000	-2.436510000	N	0.380350000	2.099650000	-1.648690000
C	-0.856190000	-2.747620000	-3.436510000	C	-0.339650000	3.009650000	-3.608680000
H	-1.256190000	-3.727620000	-3.666510000	H	-0.869650000	3.029650000	-4.548680000
C	0.003810000	-0.787620000	-3.746510000	C	0.530350000	3.419650000	-1.698680000
H	0.303810000	0.112380000	-4.266510000	H	0.880350000	4.029650000	-0.878680000
N	-0.586190000	-1.797620000	-4.406510000	N	0.110350000	4.039650000	-2.808680000
H	-0.756190000	-1.857620000	-5.406510000	H	0.080350000	5.049650000	-2.888680000
C	-1.186190000	-3.167620000	1.503490000	C	-1.899650000	-1.640350000	-2.688690000
O	-0.206190000	-3.327620000	2.223490000	O	-1.239650000	-2.600350000	-3.098690000
N	-2.386190000	-3.727620000	1.703490000	N	-3.219650000	-1.740350000	-2.508690000
H	-3.196190000	-3.467620000	1.153490000	H	-3.709650000	-0.920350000	-2.178680000
C	-2.616190000	-4.437620000	2.933490000	C	-4.169650000	-2.750350000	-2.908680000
H	-2.956190000	-5.437620000	2.653490000	H	-4.779650000	-2.290350000	-3.688690000
H	-1.756190000	-4.487620000	3.603490000	H	-3.549650000	-3.550350000	-3.298680000
C	-3.726190000	-3.777620000	3.753490000	C	-4.959650000	-3.400350000	-1.768680000
O	-4.486190000	-4.347620000	4.533490000	O	-6.019650000	-3.950350000	-2.048680000
N	-3.676190000	-2.447620000	3.713490000	N	-4.429650000	-3.350350000	-0.548680000
H	-2.866190000	-2.037620000	3.273490000	H	-3.509650000	-2.930350000	-0.518680000
C	-4.596190000	-1.577620000	4.423490000	C	-5.019650000	-3.850350000	0.671310000
H	-4.506190000	-1.867620000	5.463490000	H	-5.239650000	-4.900350000	0.541320000
C	-4.146190000	-0.117620000	4.253490000	C	-3.879650000	-3.760350000	1.681320000
H	-4.706190000	0.552380000	4.903490000	H	-4.099650000	-4.400350000	2.531320000
H	-3.136190000	0.042380000	4.633490000	H	-3.099650000	-4.330350000	1.171310000
C	-4.266190000	0.442380000	2.833490000	C	-3.439650000	-2.380350000	2.161320000
H	-5.116190000	0.042380000	2.283490000	H	-4.289650000	-1.780350000	2.491310000
H	-4.406190000	1.512380000	2.983490000	H	-2.939650000	-2.430350000	3.131310000
C	-3.046190000	0.452380000	1.933490000	C	-2.789650000	-1.540350000	1.071320000
O	-3.076190000	0.982380000	0.803490000	O	-3.019650000	-0.310350000	1.001320000
O	-1.976190000	0.002380000	2.393490000	O	-1.899650000	-2.100350000	0.391320000
C	-6.056190000	-1.697620000	4.013490000	C	-6.359650000	-3.240350000	1.091320000
O	-6.953008770	-1.163196070	4.716112030	O	-6.936472800	-3.645893730	2.133615690
N	6.393810000	0.622380000	-3.116510000	N	6.660350000	2.489650000	-1.078690000
H	6.587149580	-0.130516100	-2.487409630	H	6.607405500	1.795816330	-1.796876410
C	5.253810000	1.482380000	-2.886510000	C	5.560350000	2.649650000	-0.138680000
H	5.113810000	2.152380000	-3.736510000	H	5.710350000	3.589650000	0.391320000
C	3.963810000	0.672380000	-2.746510000	C	4.150350000	2.509650000	-0.718680000
H	3.973810000	-0.047620000	-3.566510000	H	4.100350000	3.119650000	-1.618690000
H	4.003810000	0.132380000	-1.796510000	H	4.190350000	1.449650000	-0.958680000
C	2.663810000	1.422380000	-2.846510000	C	3.090350000	2.869650000	0.291320000
N	1.563810000	1.442380000	-1.986510000	N	2.030350000	2.049650000	0.651310000
C	2.473810000	2.242380000	-3.916510000	C	3.060350000	4.039650000	0.991310000
H	3.103810000	2.362380000	-4.786510000	H	3.740350000	4.869650000	0.851310000
C	0.763810000	2.372380000	-2.516510000	C	1.350350000	2.729650000	1.591320000
H	-0.006190000	2.762380000	-1.866510000	H	0.390350000	2.429650000	1.981320000
N	1.303810000	2.912380000	-3.616510000	N	1.930350000	3.929650000	1.771320000
H	0.933810000	3.692380000	-4.146510000	H	1.520350000	4.669650000	2.321320000
C	5.483810000	2.212380000	-1.576510000	C	5.780350000	1.489650000	0.821320000
O	5.324370680	1.609186640	-0.483666260	O	5.473614280	0.319399210	0.474914380
N	4.753810000	4.272380000	1.293490000	N	5.350350000	-0.620350000	3.791320000
H	4.808281450	3.284141030	1.436376660	H	5.516319520	-1.038350710	2.910199600
C	3.803810000	4.842380000	2.223490000	C	4.310350000	-1.120350000	4.661320000
H	3.033810000	5.432380000	1.733490000	H	3.690350000	-0.320350000	5.071320000
C	3.133810000	3.682380000	2.963490000	C	3.300350000	-1.990350000	3.921310000

H	3.863810000	2.982380000	3.373490000	H	3.880350000	-2.690350000	3.311310000
H	2.503810000	4.102380000	3.733490000	H	2.670350000	-2.630350000	4.541320000
C	2.243810000	2.842380000	2.073490000	C	2.340350000	-1.280350000	3.011310000
N	0.973810000	3.252380000	1.733490000	N	1.060350000	-0.910350000	3.401310000
H	0.563810000	4.072380000	2.153490000	H	0.600350000	-1.060350000	4.281320000
C	2.363810000	1.632380000	1.453490000	C	2.400350000	-0.980350000	1.681320000
H	3.283810000	1.082380000	1.383490000	H	3.230350000	-0.970350000	0.981320000
C	0.343810000	2.232380000	1.123490000	C	0.320350000	-0.700350000	2.301320000
H	-0.686190000	2.272380000	0.803490000	H	-0.699650000	-0.350350000	2.321320000
N	1.183810000	1.242380000	0.813490000	N	1.120350000	-0.640350000	1.231320000
C	4.603810000	5.602380000	3.263490000	C	4.910350000	-2.000350000	5.751320000
O	5.714815820	5.156890500	3.651788500	O	5.719403820	-2.914981760	5.447262080
Cu	0.633810000	0.062380000	-0.706510000	Cu	0.830350000	0.679650000	-0.288680000
O	-1.916190000	1.422380000	-4.136510000	O	1.900350000	-4.770350000	0.681320000
H	-2.516190000	1.232380000	-4.856510000	H	1.030350000	-4.620350000	0.311310000
H	-2.116190000	2.312380000	-3.876510000	H	2.130350000	-5.660350000	0.411320000
O	-4.156190000	0.062380000	-2.656510000	O	-4.759650000	0.079650000	-0.828690000
H	-3.526190000	0.732380000	-2.916510000	H	-5.009650000	0.999650000	-0.788680000
H	-5.006190000	0.402380000	-2.946510000	H	-4.149650000	-0.040350000	-0.098690000
O	-2.096190000	4.072380000	-3.246510000	O	-3.499650000	1.049650000	3.191320000
H	-2.986190000	3.992380000	-3.596510000	H	-3.719650000	1.939650000	2.931320000
H	-1.616190000	4.552380000	-3.916510000	H	-3.179650000	0.629650000	2.391320000
O	-0.086190000	-0.867620000	4.233490000	O	1.530350000	-2.240350000	-2.898690000
H	0.763810000	-0.807620000	3.783490000	H	1.860350000	-3.100350000	-2.638680000
H	-0.716190000	-0.587620000	3.573490000	H	0.810350000	-2.440350000	-3.498680000
O	-3.796190000	3.622380000	0.573490000	O	-1.369650000	1.439650000	0.391320000
H	-4.346190000	3.702380000	-0.206510000	H	-2.099650000	0.809650000	0.431320000
H	-3.306190000	2.812380000	0.443490000	H	-1.769650000	2.269650000	0.641320000
O	-5.446190000	-0.137620000	-0.186510000	O	-1.049650000	1.969650000	3.921310000
H	-4.706190000	0.132380000	0.353490000	H	-1.309650000	2.889650000	3.921310000
H	-5.096190000	-0.147620000	-1.076510000	H	-1.869650000	1.479650000	3.961320000
O	5.263810000	-0.327620000	1.143490000	O	-3.479650000	2.389650000	-3.178680000
H	5.173810000	0.132380000	1.983490000	H	-3.609650000	2.509650000	-2.238690000
H	5.363810000	0.382380000	0.503490000	H	-3.719650000	1.479650000	-3.348690000
O	-1.506190000	0.922380000	-1.106510000	O	-0.849650000	-4.400350000	-0.218680000
H	-2.236190000	0.922380000	-0.486510000	H	-1.639650000	-4.810350000	-0.568680000
H	-1.896190000	0.622380000	-1.926510000	H	-1.129650000	-3.530350000	0.071320000
O	6.733810000	-1.347620000	-1.226510000	O	-2.159650000	4.019650000	0.691320000
H	6.563810000	-2.257620000	-1.436510000	H	-2.879650000	4.499650000	0.261310000
H	6.143810000	-1.147620000	-0.496510000	H	-2.159650000	4.349650000	1.591320000
O	-1.626190000	4.762380000	-0.566510000	H	-6.805668240	-2.469212550	0.498601890
H	-2.386190000	4.642380000	0.013490000	H	6.195857540	1.669036390	1.790894140
H	-1.956190000	4.542380000	-1.436510000	H	7.468916840	3.073574960	-1.006224090
O	-3.826190000	-2.057620000	-4.426510000	H	5.873222440	0.190376110	4.054108910
H	-4.616190000	-1.757620000	-4.886510000	H	4.643689530	-1.840509230	6.775157450
H	-3.756190000	-1.457620000	-3.676510000				
O	-1.606190000	2.322380000	3.913490000				
H	-0.776190000	2.612380000	3.533490000				
H	-1.756190000	1.462380000	3.523490000				
H	4.223665090	6.517475000	3.667211420				
H	4.455941120	4.457868690	0.357077660				
H	5.781585580	3.240096400	-1.581867730				
H	6.988629050	0.780700290	-3.904624830				
H	-6.320578680	-2.236439360	3.127672680				
Frame 11:				Frame 12:			
N	-0.347330000	-0.973580000	-0.224410000	N	-0.441840000	-0.990620000	-0.493800000
H	-0.987330000	-0.943580000	0.555580000	H	-1.121840000	-0.730620000	0.206200000
H	0.102670000	-1.803580000	0.155580000	H	0.008160000	-1.810620000	-0.133800000
C	-1.337330000	-1.383590000	-1.194420000	C	-1.211840000	-1.570620000	-1.573800000
H	-2.077330000	-0.593580000	-1.114420000	H	-2.061840000	-0.980620000	-1.913800000
C	-0.777330000	-1.393580000	-2.624420000	C	-0.231840000	-1.890620000	-2.713800000
H	-0.017330000	-2.113580000	-2.884410000	H	0.648160000	-2.440620000	-2.373800000
H	-1.607330000	-1.693580000	-3.274420000	H	-0.791840000	-2.470620000	-3.443800000
C	-0.557330000	0.016420000	-3.114420000	C	0.088160000	-0.630620000	-3.463800000
N	0.282670000	0.876420000	-2.414420000	N	0.618160000	0.469380000	-2.793800000
C	-1.157330000	0.606420000	-4.194420000	C	-0.181840000	-0.300620000	-4.773800000

H	-1.837330000	0.106420000	-4.864420000	H	-0.551840000	-0.810620000	-5.643800000
C	0.172670000	1.986420000	-3.144420000	C	0.568160000	1.459380000	-3.683800000
H	0.622660000	2.896420000	-2.794410000	H	0.878160000	2.469380000	-3.473800000
N	-0.557330000	1.846420000	-4.264420000	N	0.088160000	1.049380000	-4.873800000
H	-0.817330000	2.616410000	-4.874420000	H	-0.121840000	1.639380000	-5.663800000
C	-1.897330000	-2.703590000	-0.684420000	C	-1.791840000	-2.880620000	-1.073800000
O	-1.107330000	-3.603580000	-0.414420000	O	-1.041840000	-3.720620000	-0.583800000
N	-3.217330000	-2.863580000	-0.544410000	N	-3.131840000	-2.930620000	-0.983800000
H	-3.757330000	-2.103580000	-0.944420000	H	-3.541840000	-2.100620000	-1.373800000
C	-3.917330000	-3.953590000	0.105580000	C	-4.031840000	-4.000620000	-0.613800000
H	-4.767330000	-4.293590000	-0.484420000	H	-4.621840000	-4.360620000	-1.453800000
H	-3.317330000	-4.793590000	0.445580000	H	-3.401840000	-4.820620000	-0.293800000
C	-4.617330000	-3.523580000	1.385580000	C	-4.971840000	-3.570620000	0.506200000
O	-5.097330000	-4.413580000	2.085580000	O	-5.901840000	-4.300620000	0.826200000
N	-4.607330000	-2.243580000	1.755580000	N	-4.711840000	-2.490620000	1.246200000
H	-4.077330000	-1.643580000	1.135580000	H	-3.911840000	-1.910620000	1.046200000
C	-5.227330000	-1.733580000	2.955590000	C	-5.461840000	-1.950620000	2.366200000
H	-5.607330000	-2.643580000	3.435580000	H	-5.511840000	-2.730620000	3.126200000
C	-4.247330000	-1.053580000	3.905580000	C	-4.551840000	-0.880620000	2.966200000
H	-4.737330000	-0.973580000	4.875580000	H	-5.021840000	-0.460620000	3.856200000
H	-3.467330000	-1.793590000	4.075580000	H	-3.601840000	-1.290620000	3.306200000
C	-3.617330000	0.286420000	3.505580000	C	-4.231840000	0.329380000	2.086200000
H	-4.407330000	1.016420000	3.315580000	H	-5.121840000	0.749380000	1.606200000
H	-2.997330000	0.746420000	4.275590000	H	-4.001840000	1.129380000	2.786200000
C	-2.787340000	0.316420000	2.235580000	C	-3.191840000	0.209380000	0.976200000
O	-2.637330000	1.396420000	1.635580000	O	-3.321840000	0.939380000	-0.033800000
O	-2.267330000	-0.743580000	1.815580000	O	-2.321840000	-0.650620000	1.196200000
C	-6.487330000	-0.913580000	2.715580000	C	-6.831840000	-1.430620000	1.986200000
O	-7.119107720	-0.430742910	3.690923950	O	-7.736280000	-1.345390000	2.857000000
N	5.952670000	2.016420000	-3.554420000	N	6.508160000	0.649380000	-3.133800000
H	5.802248750	1.040329770	-3.711331780	H	5.931150000	-0.039190000	-3.573030000
C	5.212660000	2.436420000	-2.384410000	C	5.738160000	1.349380000	-2.113800000
H	5.532670000	3.466420000	-2.264420000	H	6.068160000	2.349380000	-1.853800000
C	3.702670000	2.296410000	-2.604420000	C	4.268160000	1.399380000	-2.553800000
H	3.442670000	2.856420000	-3.504420000	H	4.228160000	1.909380000	-3.513800000
H	3.492670000	1.276420000	-2.924420000	H	3.918160000	0.369380000	-2.653800000
C	2.782670000	2.826420000	-1.544410000	C	3.428160000	2.309380000	-1.713800000
N	2.092670000	2.076420000	-0.594420000	N	2.328160000	1.919380000	-0.943800000
C	2.582670000	4.166420000	-1.344420000	C	3.618160000	3.659380000	-1.613800000
H	2.982670000	5.036420000	-1.844420000	H	4.348160000	4.299380000	-2.083800000
C	1.582670000	2.976420000	0.245580000	C	1.888160000	3.049380000	-2.553800000
H	0.932670000	2.756420000	1.075580000	H	1.028160000	3.219380000	0.246200000
N	1.712660000	4.206410000	-0.274420000	N	2.508160000	4.119380000	-0.923800000
H	1.252670000	5.036420000	0.095580000	H	2.248160000	5.069380000	-0.703800000
C	5.612670000	1.566420000	-1.204420000	C	5.868160000	0.509380000	-0.853800000
O	4.965561870	0.518143430	-0.947636310	O	5.231260000	-0.570900000	-0.749290000
N	6.182670000	0.486420000	2.265580000	N	5.398160000	-0.030620000	3.216200000
H	6.701828590	-0.351697450	2.098147950	H	5.570620000	-0.916270000	2.785160000
C	5.462660000	0.366410000	3.515580000	C	4.508160000	0.059380000	4.356200000
H	4.952670000	1.276420000	3.835580000	H	4.238160000	1.109380000	4.356200000
C	4.472670000	-0.803580000	3.515580000	C	3.278160000	-0.820620000	4.106200000
H	4.932670000	-1.703590000	3.115590000	H	3.508160000	-1.880620000	3.996200000
H	4.312670000	-1.173580000	4.535580000	H	2.658160000	-0.800620000	4.996200000
C	3.162670000	-0.483580000	2.855580000	C	2.328160000	-0.340620000	3.046200000
N	2.112670000	0.066420000	3.565580000	N	1.068160000	0.109380000	3.396200000
H	2.062670000	0.176420000	4.565580000	H	0.638160000	0.149380000	4.306200000
C	2.762670000	-0.443580000	1.545580000	C	2.428160000	-0.240620000	1.686200000
H	3.392670000	-0.833580000	0.765580000	H	3.288160000	-0.430620000	1.066200000
C	1.152670000	0.366410000	2.665580000	C	0.458160000	0.629380000	2.316200000
H	0.182670000	0.776420000	2.915580000	H	-0.461840000	1.199380000	2.266200000
N	1.532670000	0.186420000	1.395580000	N	1.258160000	0.399380000	1.276200000
C	6.492670000	-0.083580000	4.545580000	C	5.178160000	-0.370620000	5.666200000
O	7.267502990	-1.040071650	4.284183500	O	6.171980000	-1.142150000	5.640940000
Cu	0.892670000	0.466420000	-0.524420000	Cu	0.918160000	0.379380000	-0.793800000
O	1.702670000	0.106420000	-5.534420000	O	-0.761840000	-2.320620000	2.326200000
H	1.232670000	-0.523580000	-6.074420000	H	-1.391840000	-1.830620000	1.786200000
H	1.012670000	0.606420000	-5.094420000	H	-1.071840000	-3.220620000	2.296200000

O	-1.237330000	-2.453590000	3.605580000	O	-1.791840000	-4.780620000	1.896200000
H	-1.147330000	-2.003580000	4.445580000	H	-1.631840000	-5.710620000	1.756200000
H	-1.737330000	-1.833580000	3.065580000	H	-1.701840000	-4.390620000	1.026200000
O	4.642670000	0.016420000	-5.184420000	O	-3.131840000	4.809380000	0.146200000
H	4.772670000	-0.483580000	-5.984420000	H	-3.381840000	5.739380000	0.136200000
H	3.692670000	0.156420000	-5.144420000	H	-2.171840000	4.829380000	0.096200000
O	-4.177330000	2.756420000	-0.454420000	O	-0.851840000	1.859380000	-0.603800000
H	-3.787340000	2.396420000	0.345580000	H	-0.991840000	2.729380000	-0.963800000
H	-4.857330000	3.346420000	-0.134410000	H	-1.721840000	1.529380000	-0.393800000
O	0.142670000	-4.903580000	-2.474410000	O	-3.691840000	2.999380000	-1.653800000
H	0.242670000	-5.803580000	-2.154420000	H	-3.531840000	2.379380000	-0.943800000
H	-0.457330000	-4.493580000	-1.844420000	H	-3.731840000	3.849380000	-1.213800000
O	-4.707330000	-0.733580000	-1.724410000	O	1.478160000	-2.950620000	0.446200000
H	-5.177330000	-0.963580000	-2.524420000	H	1.628160000	-3.820620000	0.076200000
H	-4.457330000	0.186420000	-1.854420000	H	1.178160000	-3.120620000	1.336200000
O	0.312670000	3.866410000	3.945580000	O	-1.001840000	4.299380000	-2.073800000
H	-0.577330000	3.516420000	3.875580000	H	-1.741840000	3.689380000	-2.083800000
H	0.412670000	4.466420000	3.205590000	H	-1.351840000	5.109380000	-2.443800000
O	-1.077330000	1.976420000	-0.294410000	O	-0.571840000	5.839380000	0.566200000
H	-1.567330000	1.666420000	0.475580000	H	0.378160000	5.729380000	0.546200000
H	-1.667330000	2.596420000	-0.714420000	H	-0.721840000	6.729380000	0.236200000
O	-4.187330000	1.686420000	-3.874420000	O	-4.631840000	-0.650620000	-1.753800000
H	-4.817330000	1.996420000	-3.224410000	H	-4.361840000	0.069380000	-1.183800000
H	-3.457330000	2.296410000	-3.814420000	H	-4.501840000	-0.310620000	-2.643800000
O	0.492670000	-2.983580000	1.765580000	H	4.800790000	-0.014750000	6.602070000
H	-0.007330000	-2.693580000	2.515580000	H	5.840110000	0.792930000	2.860680000
H	-0.097330000	-3.573580000	1.295580000	H	6.826190000	1.304270000	-3.819350000
O	-2.117330000	4.366410000	-1.684420000	H	6.501230000	0.836570000	-0.055630000
H	-1.907330000	4.826420000	-0.874420000	H	-7.031140000	-1.135550000	0.977180000
H	-3.027330000	4.106420000	-1.584420000				
O	-2.287340000	3.676420000	3.125580000				
H	-2.427330000	4.476420000	2.615590000				
H	-2.467330000	2.966420000	2.505580000				
H	6.927834880	2.184443320	-3.410122990				
H	-6.835732130	-0.747790750	1.717567030				
H	6.444551030	1.845172850	-0.591908120				
H	6.556739990	0.413891650	5.490734480				
H	6.810604820	1.263061760	2.315833730				
Frame 13:				Frame 14:			
N	-0.448770000	-1.047540000	-0.210270000	N	0.092460000	-1.372990000	-0.001200000
H	-0.868770000	-1.007540000	0.709740000	H	-0.037540000	-1.192990000	0.988800000
H	-0.068770000	-1.977540000	-0.110260000	H	1.082460000	-1.572990000	0.058800000
C	-1.638770000	-1.527540000	-0.880260000	C	-0.657540000	-2.602990000	-0.051200000
H	-2.468770000	-0.907540000	-0.540260000	H	-1.617540000	-2.512990000	0.468800000
C	-1.528770000	-1.417540000	-2.410260000	C	-0.947540000	-3.092990000	-1.471200000
H	-0.728770000	-2.077540000	-2.730260000	H	-0.047540000	-3.072990000	-2.091200000
H	-2.408770000	-1.867540000	-2.860260000	H	-1.307540000	-4.102990000	-1.611200000
C	-1.328770000	-0.017540000	-2.930260000	C	-1.857540000	-2.172990000	-2.241200000
N	-0.278770000	0.832460000	-2.620270000	N	-1.717540000	-0.792990000	-2.201200000
C	-2.238770000	0.662460000	-3.700260000	C	-2.897540000	-2.532990000	-3.061200000
H	-3.188770000	0.272460000	-4.050260000	H	-3.327540000	-3.462990000	-3.391200000
C	-0.438770000	1.922460000	-3.380260000	C	-2.747540000	-0.372990000	-2.951200000
H	0.231230000	2.762450000	-3.460270000	H	-3.007540000	0.657010000	-3.131200000
N	-1.608770000	1.842460000	-4.040260000	N	-3.427540000	-1.352990000	-3.551200000
H	-1.968770000	2.542460000	-4.670260000	H	-4.177540000	-1.272990000	-4.221200000
C	-1.948770000	-2.947540000	-0.430260000	C	0.072460000	-3.682990000	0.748800000
O	-1.048770000	-3.727540000	-0.120270000	O	1.242460000	-3.902990000	0.428800000
N	-3.238770000	-3.287540000	-0.340260000	N	-0.507540000	-4.322990000	1.758800000
H	-3.968770000	-2.617540000	-0.550260000	H	-1.477540000	-4.092990000	1.938800000
C	-3.778770000	-4.477540000	0.289730000	C	0.052460000	-5.282990000	2.688800000
H	-4.598770000	-4.917540000	-0.270260000	H	-0.647540000	-6.092990000	2.918800000
H	-3.158770000	-5.357540000	0.449740000	H	1.002460000	-5.742990000	2.428800000
C	-4.448770000	-4.147550000	1.619740000	C	0.162460000	-4.692990000	4.088800000
O	-5.288770000	-4.927540000	2.059740000	O	1.242460000	-4.902990000	4.628800000
N	-4.158770000	-3.017540000	2.279740000	N	-0.807540000	-3.902990000	4.568800000
H	-3.478770000	-2.357540000	1.949740000	H	-1.617540000	-3.752990000	3.978800000

C	-4.728770000	-2.697540000	3.569740000	C	-0.747540000	-3.062990000	5.738800000
H	-4.558770000	-3.517540000	4.269740000	H	-0.177540000	-3.772990000	6.328800000
C	-3.688770000	-1.767540000	4.209740000	C	-0.027540000	-1.722990000	5.538800000
H	-4.048770000	-1.537540000	5.209740000	H	0.202460000	-1.452990000	6.568800000
H	-2.738770000	-2.297540000	4.279740000	H	0.932460000	-1.862990000	5.038800000
C	-3.518770000	-0.367540000	3.609740000	C	-0.817540000	-0.562990000	4.928800000
H	-4.468770000	0.152460000	3.489740000	H	-1.867540000	-0.512990000	5.188800000
H	-3.158770000	0.342460000	4.359740000	H	-0.377540000	0.397010000	5.178800000
C	-2.668770000	-0.277540000	2.349740000	C	-0.827540000	-0.592990000	3.398800000
O	-2.808770000	0.712460000	1.609740000	O	-1.907540000	-0.232990000	2.878800000
O	-1.858770000	-1.197540000	2.129730000	O	0.192460000	-0.892990000	2.738800000
C	-6.158770000	-2.167540000	3.579740000	C	-2.087540000	-2.992990000	6.458800000
O	-6.709841060	-1.864416340	4.669697470	O	-2.248760000	-2.186290000	7.411070000
N	5.401230000	1.792460000	-4.260260000	N	1.502460000	1.617010000	-6.521200000
H	5.330737260	0.795517770	-4.293978820	H	2.164730000	0.925240000	-6.233340000
C	4.741230000	2.282460000	-3.070260000	C	0.932460000	2.257010000	-5.351200000
H	4.911230000	3.352450000	-2.990260000	H	0.432460000	3.207010000	-5.551200000
C	3.261230000	1.882460000	-3.160260000	C	-0.047540000	1.307010000	-4.671200000
H	2.981230000	2.202460000	-4.160260000	H	-0.757540000	1.017010000	-5.431200000
H	3.051230000	0.812460000	-3.050260000	H	0.442460000	0.427010000	-4.251200000
C	2.391230000	2.682460000	-2.230260000	C	-0.797540000	2.067010000	-3.611200000
N	1.811230000	2.192450000	-1.070260000	N	-0.607540000	1.847010000	-2.241200000
C	2.171230000	4.032460000	-2.290260000	C	-1.847540000	2.937010000	-3.711200000
H	2.511230000	4.782460000	-2.990260000	H	-2.427540000	3.337010000	-4.521200000
C	1.441230000	3.292460000	-0.410260000	C	-1.447540000	2.627010000	-1.561200000
H	0.931230000	3.282460000	0.539730000	H	-1.527540000	2.697010000	-0.491200000
N	1.591230000	4.442450000	-1.100260000	N	-2.317540000	3.177010000	-2.431200000
H	1.161230000	5.322460000	-0.870270000	H	-3.147540000	3.697010000	-2.191200000
C	5.411230000	1.632460000	-1.870270000	C	2.202460000	2.487010000	-4.541200000
O	4.986199030	0.532159040	-1.431798750	O	2.629960000	1.587210000	-3.772330000
N	6.051230000	1.452460000	1.749740000	N	4.352460000	4.167010000	-1.831200000
H	6.087650740	0.579076310	1.264049750	H	5.301270000	4.037120000	-2.119100000
C	5.511230000	1.512450000	3.089740000	C	4.322460000	4.607010000	-0.451200000
H	4.981230000	2.432460000	3.329740000	H	3.482460000	5.267010000	-0.221200000
C	4.541230000	0.362460000	3.349740000	C	4.052460000	3.387010000	0.428800000
H	4.951230000	-0.637540000	3.229740000	H	4.892460000	2.687010000	0.398800000
H	4.351230000	0.422460000	4.419740000	H	4.082460000	3.787010000	1.438800000
C	3.221230000	0.392460000	2.639740000	C	2.722460000	2.707010000	0.238800000
N	2.081230000	0.942450000	3.199740000	N	1.842460000	2.677010000	1.298800000
H	2.131230000	1.312460000	4.139740000	H	1.942460000	3.267010000	2.118800000
C	2.851230000	0.182460000	1.339740000	C	2.332460000	1.717010000	-0.631200000
H	3.441230000	-0.077540000	0.469730000	H	2.772460000	1.337010000	-1.551200000
C	1.111230000	0.962460000	2.279740000	C	0.912460000	1.747010000	1.038800000
H	0.161230000	1.362460000	2.609740000	H	0.032460000	1.557010000	1.628800000
N	1.521230000	0.502460000	1.099740000	N	1.162460000	1.147010000	-0.131200000
C	6.591230000	1.382460000	4.159740000	C	5.622460000	5.267010000	-0.001200000
O	7.610242920	0.676708990	3.942717570	O	6.662620000	5.148980000	-0.699560000
Cu	0.601230000	0.532460000	-0.760260000	Cu	-0.257540000	0.137010000	-1.171200000
O	-0.848770000	4.102450000	2.569740000	O	2.582460000	-1.462990000	2.388800000
H	-1.138770000	4.992460000	2.409740000	H	2.902460000	-2.082990000	3.038800000
H	-1.648770000	3.612460000	2.759740000	H	1.652460000	-1.362990000	2.578800000
O	-1.908770000	4.142460000	-1.430260000	O	-4.517540000	-0.232990000	2.918800000
H	-1.668770000	4.262450000	-2.350260000	H	-3.567540000	-0.092990000	2.938800000
H	-2.118770000	5.022460000	-1.120270000	H	-4.877540000	0.507010000	3.418800000
O	-3.318770000	2.802460000	3.219730000	O	-2.777540000	2.337010000	3.508800000
H	-3.198770000	2.062460000	2.629730000	H	-2.567540000	1.497010000	3.098800000
H	-4.058770000	3.282460000	2.849740000	H	-3.557540000	2.157010000	4.028800000
O	3.581230000	-2.777540000	-0.410260000	O	-4.177540000	-1.462990000	0.208800000
H	3.561230000	-3.697540000	-0.660260000	H	-4.587540000	-0.782990000	0.758800000
H	3.031230000	-2.717540000	0.369740000	H	-4.907540000	-1.852990000	-0.261200000
O	-4.948770000	1.802460000	-2.950260000	O	-1.957540000	0.347010000	0.338800000
H	-5.218770000	0.972460000	-3.330260000	H	-1.887540000	0.147010000	1.278800000
H	-4.618770000	1.572460000	-2.080260000	H	-2.817540000	0.027010000	0.088800000
O	-1.018770000	1.972460000	-0.040260000	H	5.649680000	5.830200000	0.908180000
H	-1.348770000	2.852450000	-0.240260000	H	3.919840000	4.857640000	-2.410740000
H	-1.698770000	1.582460000	0.499740000	H	1.961140000	2.302910000	-7.086130000
O	1.461230000	-2.947540000	1.259740000	H	2.730760000	3.413610000	-4.626180000

H	1.281230000	-2.467540000	2.069740000	H	-2.892010000	-3.629720000	6.155010000
H	0.781230000	-3.617540000	1.219730000				
O	-4.378770000	1.632460000	-0.290260000				
H	-4.488770000	2.572460000	-0.100260000				
H	-3.918770000	1.292460000	0.479740000				
O	-0.178770000	-2.397550000	3.959740000				
H	-0.538770000	-1.977540000	4.739740000				
H	-0.668770000	-2.017540000	3.229740000				
H	6.244173060	2.110561410	-1.398544560				
H	6.365125400	2.057978550	-4.240121350				
H	6.388458510	2.284254670	1.308803930				
H	6.482129250	1.891394560	5.094610380				
H	-6.693486900	-2.053434960	2.659980310				
Frame 15:				Frame 16:			
N	-0.365210000	-1.271190000	0.304870000	N	-1.032390000	-1.180980000	0.371490000
H	0.094790000	-1.071190000	1.184870000	H	-0.532390000	-1.360980000	1.221490000
H	0.354790000	-1.951190000	0.084870000	H	-1.102400000	-2.110980000	-0.018510000
C	-1.425210000	-2.021190000	0.934870000	C	-2.362390000	-1.280980000	0.941490000
H	-1.985210000	-1.361190000	1.604870000	H	-2.562390000	-0.410980000	1.561490000
C	-2.375210000	-2.591190000	-0.115130000	C	-3.352400000	-1.300980000	-0.218510000
H	-1.855210000	-3.081190000	-0.945130000	H	-3.042390000	-2.110980000	-0.878510000
H	-2.965210000	-3.371190000	0.364870000	H	-4.342390000	-1.440980000	0.211490000
C	-3.215210000	-1.521190000	-0.735130000	C	-3.452390000	-0.020980000	-1.008510000
N	-2.725210000	-0.281190000	-1.165130000	N	-2.352400000	0.789020000	-1.298510000
C	-4.565210000	-1.511190000	-0.975130000	C	-4.602400000	0.509020000	-1.518510000
H	-5.285210000	-2.261190000	-0.675130000	H	-5.632390000	0.179020000	-1.458510000
C	-3.775210000	0.468810000	-1.495130000	C	-2.852400000	1.889020000	-1.868510000
H	-3.735210000	1.508810000	-1.805130000	H	-2.342390000	2.829020000	-2.038510000
N	-4.915210000	-0.231190000	-1.365130000	N	-4.182390000	1.749020000	-1.958510000
H	-5.885210000	-0.031190000	-1.545130000	H	-4.752390000	2.539020000	-2.198510000
C	-0.685210000	-3.111190000	1.684870000	C	-2.452390000	-2.540980000	1.791490000
O	0.044790000	-3.941190000	1.144870000	O	-2.122390000	-3.600980000	1.261490000
N	-1.055210000	-3.071190000	2.974870000	N	-2.842390000	-2.490980000	3.071490000
H	-1.805210000	-2.501190000	3.334870000	H	-2.892390000	-1.570980000	3.471490000
C	-0.525210000	-3.921190000	4.024870000	C	-2.862390000	-3.600980000	4.001490000
H	-1.355210000	-4.581190000	4.254870000	H	-3.902390000	-3.760980000	4.281490000
H	0.234790000	-4.551190000	3.554870000	H	-2.462390000	-4.530980000	3.571490000
C	0.104790000	-3.081190000	5.124870000	C	-2.022390000	-3.260980000	5.221490000
O	0.364790000	-3.681190000	6.174870000	O	-2.392390000	-3.630980000	6.331490000
N	0.474790000	-1.821190000	4.904870000	N	-0.952390000	-2.490980000	5.031490000
H	0.214790000	-1.371190000	4.034870000	H	-0.752390000	-2.150980000	4.101490000
C	1.434790000	-1.051190000	5.664870000	C	-0.002390000	-2.220980000	6.101490000
H	2.014790000	-1.801190000	6.204870000	H	0.187610000	-3.110980000	6.681490000
C	2.444790000	-0.281190000	4.814870000	C	1.257610000	-1.900980000	5.291490000
H	3.244790000	0.118810000	5.434870000	H	1.997610000	-2.040980000	6.081490000
H	2.944790000	-0.941190000	4.104870000	H	1.507610000	-2.660980000	4.551490000
C	1.914790000	0.968810000	4.104870000	C	1.447610000	-0.470980000	4.781490000
H	1.504790000	1.748810000	4.734870000	H	1.177610000	0.289020000	5.521490000
H	2.814790000	1.408810000	3.674870000	H	2.487600000	-0.220980000	4.571490000
C	0.834790000	0.718810000	3.064870000	C	0.697610000	-0.230980000	3.481490000
O	0.014790000	1.628810000	2.804870000	O	0.187610000	0.909020000	3.361490000
O	0.934790000	-0.331190000	2.384870000	O	0.387610000	-1.160980000	2.711490000
C	0.874790000	-0.081190000	6.704870000	C	-0.402390000	-1.140980000	7.091490000
O	1.652340000	0.675030000	7.342930000	O	0.341520000	-0.879700000	8.072250000
N	-0.845210000	-1.081190000	-6.585130000	N	0.287610000	0.849020000	-6.748510000
H	-1.296820000	-1.807390000	-6.066800000	H	-0.276260000	0.072400000	-6.467580000
C	-0.665210000	0.078810000	-5.735130000	C	0.857610000	1.479020000	-5.578510000
H	-0.905210000	1.018810000	-6.225130000	H	1.067610000	2.539020000	-5.748510000
C	-1.505210000	-0.131190000	-4.465130000	C	-0.132390000	1.369020000	-4.418510000
H	-2.525210000	-0.451190000	-4.715130000	H	-1.152390000	1.569020000	-4.748510000
H	-1.115210000	-0.831190000	-3.735130000	H	-0.182390000	0.389020000	-3.968510000
C	-1.625210000	1.158810000	-3.695130000	C	0.107610000	2.359020000	-3.308510000
N	-0.965210000	1.388810000	-2.495130000	N	0.177610000	1.959020000	-1.978510000
C	-2.265210000	2.288810000	-4.125130000	C	0.307610000	3.709020000	-3.358510000
H	-2.755210000	2.498810000	-5.065130000	H	0.197610000	4.379020000	-4.198510000
C	-1.185210000	2.678810000	-2.215130000	C	0.377610000	3.059020000	-1.248510000

H	-0.675210000	3.288810000	-1.485130000	H	0.667610000	3.079020000	-0.208510000
N	-1.955210000	3.228810000	-3.175130000	N	0.457610000	4.129020000	-2.048510000
H	-2.125210000	4.218810000	-3.325130000	H	0.487600000	5.109020000	-1.798510000
C	0.814790000	0.158810000	-5.425130000	C	2.067610000	0.619020000	-5.248510000
O	1.334600000	-0.659040000	-4.622340000	O	1.910320000	-0.511810000	-4.719310000
N	4.114790000	1.638810000	-4.215130000	N	5.027610000	-0.100980000	-3.138510000
H	4.717090000	0.840680000	-4.229670000	H	5.141710000	-1.033970000	-3.479830000
C	4.544790000	2.548810000	-3.175130000	C	5.627610000	0.009020000	-1.818510000
H	3.864790000	3.388810000	-3.015130000	H	5.547610000	1.009020000	-1.398510000
C	4.614790000	1.778810000	-1.855130000	C	4.967610000	-1.100980000	-1.008510000
H	5.224790000	0.888810000	-2.015130000	H	4.867610000	-2.060980000	-1.518510000
H	5.114790000	2.368810000	-1.095130000	H	5.527610000	-1.240980000	-0.078510000
C	3.254790000	1.438810000	-1.305130000	C	3.587610000	-0.720980000	-0.538510000
N	2.674790000	2.278810000	-0.375130000	N	3.527610000	0.079020000	0.591490000
H	3.014790000	3.138810000	0.034870000	H	4.277610000	0.499020000	1.131490000
C	2.354790000	0.448810000	-1.585130000	C	2.317610000	-0.840980000	-1.008510000
H	2.484790000	-0.411190000	-2.215130000	H	1.917610000	-1.250980000	-1.938510000
C	1.454790000	1.768810000	-0.145130000	C	2.237600000	0.379020000	0.791490000
H	0.714790000	2.288810000	0.434870000	H	1.797610000	0.969020000	1.581490000
N	1.164790000	0.698810000	-0.885130000	N	1.467610000	-0.130980000	-0.178510000
C	5.904790000	3.058810000	-3.635130000	C	7.087610000	-0.410980000	-1.908510000
O	6.679110000	2.298730000	-4.272520000	O	7.407870000	-1.437550000	-2.562080000
Cu	-0.745210000	0.018810000	-1.105130000	Cu	-0.432390000	0.279020000	-0.768510000
O	0.054790000	4.198810000	2.594870000	O	-1.732390000	4.119020000	1.051490000
H	-0.525210000	4.498810000	3.294870000	H	-1.132390000	4.819020000	0.771490000
H	0.094790000	3.248810000	2.714870000	H	-2.052390000	4.399020000	1.901490000
O	-2.075210000	2.308810000	4.134870000	O	-0.702390000	1.649020000	1.011490000
H	-1.185210000	2.288810000	3.774870000	H	-0.342390000	1.359020000	1.851490000
H	-2.145210000	3.168810000	4.554870000	H	-1.132390000	2.479020000	1.221490000
O	2.494790000	-2.211190000	1.994870000	O	1.157610000	3.199020000	4.081490000
H	2.444790000	-2.721190000	2.804870000	H	0.487600000	3.649020000	4.591490000
H	1.904790000	-1.461190000	2.144870000	H	0.777610000	2.339020000	3.891490000
O	-1.425210000	1.298810000	0.634870000	O	-2.362390000	0.469020000	3.841490000
H	-1.035210000	1.398810000	1.504870000	H	-1.442390000	0.699020000	3.731490000
H	-2.245210000	1.788810000	0.684870000	H	-2.812390000	1.309020000	3.941490000
O	-3.845210000	2.368810000	0.714870000	O	-4.562390000	1.269020000	1.831490000
H	-4.445210000	2.558810000	-0.005130000	H	-3.822390000	1.859020000	1.991490000
H	-3.845210000	3.168810000	1.244870000	H	-5.002390000	1.629020000	1.061490000
O	-3.345210000	-1.411190000	3.954870000	O	0.967610000	-3.460980000	1.621490000
H	-3.475210000	-0.661190000	3.374870000	H	0.797610000	-4.210980000	2.191490000
H	-4.115210000	-1.951190000	3.834870000	H	0.737600000	-2.700980000	2.151490000
O	-4.105210000	1.008810000	2.954870000	H	7.841790000	0.166600000	-1.416070000
H	-3.385210000	1.618810000	3.104870000	H	5.475350000	0.539370000	-3.762600000
H	-4.335210000	1.138810000	2.034870000	H	3.052710000	0.975440000	-5.466290000
H	6.201510000	4.063270000	-3.416220000	H	1.022660000	0.528430000	-7.345940000
H	4.153870000	2.102060000	-5.100500000	H	-1.316750000	-0.602240000	6.955060000
H	-0.178390000	-0.045130000	6.890400000				
H	1.418620000	0.910750000	-5.888690000				
H	-1.409630000	-0.833140000	-7.372470000				
Frame 17:				Frame 18:			
N	-0.379490000	-1.429580000	0.147200000	N	-1.428890000	-0.233400000	-0.016600000
H	-0.019490000	-1.049580000	1.017200000	H	-1.548890000	-0.333400000	0.983400000
H	0.330510000	-2.139580000	0.097200000	H	-1.678890000	-1.203400000	-0.146610000
C	-1.619490000	-1.889580000	0.737200000	C	-2.658890000	0.466600000	-0.306610000
H	-2.179490000	-1.039580000	1.127200000	H	-2.458890000	1.396600000	0.223390000
C	-2.629490000	-2.369580000	-0.302800000	C	-2.928890000	0.916600000	-1.746600000
H	-2.119490000	-2.979580000	-1.032800000	H	-2.948890000	-0.023400000	-2.306610000
H	-3.389490000	-2.989580000	0.177200000	H	-3.948890000	1.296600000	-1.726600000
C	-3.209490000	-1.299580000	-1.192800000	C	-1.948890000	1.966600000	-2.206600000
N	-2.449490000	-0.299580000	-1.802800000	N	-0.588890000	1.646600000	-2.246600000
C	-4.549490000	-1.089580000	-1.372800000	C	-2.198890000	3.196600000	-2.746600000
H	-5.359490000	-1.629580000	-0.902800000	H	-3.118890000	3.706600000	-3.016600000
C	-3.369490000	0.380420000	-2.492800000	C	-0.048890000	2.756600000	-2.756610000
H	-3.259490000	1.250420000	-3.122800000	H	0.971110000	3.066600000	-2.896610000
N	-4.619490000	-0.029580000	-2.252800000	N	-0.958890000	3.676600000	-3.116600000
H	-5.439490000	0.420420000	-2.642800000	H	-0.848890000	4.576600000	-3.556610000

C	-1.389490000	-3.019580000	1.727210000	C	-3.898890000	-0.263400000	0.183400000
O	-0.919490000	-4.069580000	1.297200000	O	-4.258890000	-1.373400000	-0.196600000
N	-1.639490000	-2.719580000	3.007200000	N	-4.548890000	0.356600000	1.173390000
H	-2.139490000	-1.889580000	3.297200000	H	-4.248890000	1.206600000	1.633400000
C	-1.319490000	-3.739580000	3.987200000	C	-5.698890000	-0.283400000	1.783400000
H	-2.229490000	-3.829580000	4.587200000	H	-6.558890000	0.306600000	1.473390000
H	-1.139490000	-4.739580000	3.597200000	H	-5.868890000	-1.293400000	1.403390000
C	-0.229490000	-3.279580000	4.947200000	C	-5.488890000	-0.303400000	3.293400000
O	0.690510000	-4.079580000	5.147200000	O	-6.558890000	-0.333400000	3.903390000
N	-0.419490000	-2.079580000	5.497200000	N	-4.288890000	-0.193400000	3.863400000
H	-1.339490000	-1.689580000	5.337200000	H	-3.618890000	-0.423400000	3.143400000
C	0.520510000	-1.379580000	6.337200000	C	-3.818890000	-0.263400000	5.233400000
H	1.010510000	-2.209580000	6.847200000	H	-4.128890000	-1.013400000	5.653390000
C	1.610510000	-0.599580000	5.607200000	C	-2.308890000	-0.063400000	5.473390000
H	2.310510000	-0.179580000	6.327200000	H	-2.238890000	-0.053400000	6.553400000
H	2.230510000	-1.339580000	5.107200000	H	-1.918890000	-1.063400000	5.283400000
C	1.140510000	0.390420000	4.537200000	C	-1.458890000	0.996600000	4.783400000
H	0.500510000	1.180420000	4.917200000	H	-1.938890000	1.976600000	4.813390000
H	2.050510000	0.870420000	4.177200000	H	-0.478890000	1.036600000	5.253400000
C	0.740510000	-0.119580000	3.157200000	C	-1.068890000	0.706600000	3.343400000
O	1.120510000	-1.249580000	2.767200000	O	-1.558890000	-0.273400000	2.743390000
O	-0.129490000	0.550420000	2.547200000	O	-0.298890000	1.566600000	2.853390000
C	-0.199490000	-0.629580000	7.447200000	C	-4.398890000	1.146600000	5.953400000
O	0.452040000	0.099810000	8.239080000	O	-4.420480000	1.179670000	7.211180000
N	-0.929490000	0.330420000	-7.422800000	N	3.131110000	-1.013400000	-6.216600000
H	-0.545110000	-0.588300000	-7.513390000	H	2.622600000	-1.874440000	-6.220640000
C	-0.339490000	0.990420000	-6.272790000	C	3.531110000	-0.693400000	-4.856600000
H	-0.219490000	2.060420000	-6.432790000	H	4.381110000	-0.023400000	-4.856600000
C	-1.069490000	0.720420000	-4.962800000	C	2.311110000	-0.053400000	-4.186610000
H	-2.139490000	0.630420000	-5.112790000	H	1.861110000	0.666600000	-4.856600000
H	-0.819490000	-0.259580000	-4.562800000	H	1.541110000	-0.793400000	-3.976600000
C	-0.869490000	1.760420000	-3.892800000	C	2.731110000	0.726600000	-2.966600000
N	-0.529490000	1.520420000	-2.562800000	N	2.111110000	0.636600000	-1.716600000
C	-1.039490000	3.110420000	-4.032800000	C	3.691110000	1.696600000	-2.966600000
H	-1.369490000	3.750420000	-4.832800000	H	4.271110000	2.186600000	-3.736610000
C	-0.309490000	2.690420000	-1.972800000	C	2.851110000	1.486600000	-1.006610000
H	-0.169490000	3.050420000	-0.962800000	H	2.611110000	1.706600000	0.033400000
N	-0.549490000	3.670420000	-2.862790000	N	3.821110000	2.136600000	-1.666610000
H	-0.699490000	4.650420000	-2.692800000	H	4.401110000	2.886600000	-1.306610000
C	1.030510000	0.340420000	-6.122800000	C	4.031110000	-1.933400000	-4.136600000
O	1.121690000	-0.902990000	-5.951970000	O	3.220970000	-2.671580000	-3.518270000
N	4.690510000	0.590420000	-4.252800000	N	5.021110000	-3.873400000	-1.456600000
H	4.504940000	-0.371170000	-4.455060000	H	4.642750000	-4.735690000	-1.793190000
C	5.410510000	0.950420000	-3.052800000	C	4.921110000	-3.833400000	-0.016600000
H	5.120510000	1.940420000	-2.692800000	H	5.311110000	-2.863400000	0.303400000
C	5.040510000	-0.099580000	-2.002800000	C	3.471110000	-3.953400000	0.443390000
H	5.130510000	-1.109580000	-2.392800000	H	2.901110000	-4.703400000	-0.116600000
H	5.700510000	-0.009580000	-1.142800000	H	3.581110000	-4.393400000	1.443390000
C	3.680510000	0.170420000	-1.422800000	C	2.761110000	-2.623400000	0.463400000
N	3.510510000	0.820420000	-0.212800000	N	2.901110000	-1.773400000	1.533400000
H	4.280510000	1.170420000	0.327200000	H	3.311110000	-2.153400000	2.373400000
C	2.410510000	-0.139580000	-1.812800000	C	1.831110000	-2.033400000	-0.346610000
H	2.010510000	-0.659580000	-2.672800000	H	1.521110000	-2.353400000	-1.326610000
C	2.190510000	0.880420000	0.067210000	C	1.851110000	-0.933400000	1.553400000
H	1.860510000	1.520420000	0.877200000	H	1.521110000	-0.353400000	2.403390000
N	1.460510000	0.360420000	-0.922800000	N	1.201110000	-1.033400000	0.393400000
C	6.880510000	0.990420000	-3.472800000	C	5.721110000	-4.943400000	0.643400000
O	7.273290000	0.307690000	-4.454210000	O	5.765290000	-6.085600000	0.117090000
Cu	-0.499490000	-0.069580000	-1.232800000	Cu	0.281110000	0.236600000	-0.926600000
O	1.860510000	-3.129580000	0.847200000	O	-1.648890000	3.836600000	2.483400000
H	1.180510000	-3.779580000	1.027200000	H	-1.318890000	3.066600000	2.943390000
H	1.760510000	-2.479580000	1.537200000	H	-1.118890000	3.876600000	1.683400000
O	-3.759490000	1.990420000	1.237200000	O	-4.098890000	2.886600000	1.913400000
H	-3.739490000	2.910420000	0.957200000	H	-3.228890000	3.276600000	2.043400000
H	-3.489490000	2.010420000	2.157200000	H	-4.298890000	3.066600000	0.993390000
O	-1.319490000	1.130420000	0.467200000	O	0.081110000	2.146600000	0.313390000
H	-0.809490000	1.010420000	1.267200000	H	-0.098890000	1.896600000	1.223390000

H	-2.199490000	1.370420000	0.777200000	H	0.381110000	3.056600000	0.373400000
O	-2.919490000	-0.649580000	4.707200000	O	0.891110000	4.746600000	-0.066600000
H	-2.829490000	0.200420000	4.287200000	H	0.321110000	5.496600000	-0.206600000
H	-3.639490000	-1.079580000	4.247200000	H	1.631110000	5.096600000	0.433400000
O	-2.119490000	1.950420000	3.497200000	O	-1.368890000	-2.803400000	2.993390000
H	-1.359490000	1.420420000	3.247200000	H	-1.338890000	-1.853400000	3.003400000
H	-1.739490000	2.770420000	3.827200000	H	-1.968890000	-3.033400000	3.703400000
O	-3.719490000	4.490420000	-0.002800000	O	1.801110000	1.796600000	4.443390000
H	-4.129490000	4.590420000	-0.862790000	H	1.061110000	1.586600000	3.863400000
H	-3.529490000	5.390420000	0.277200000	H	1.561110000	2.636600000	4.833390000
H	7.575010000	1.598930000	-2.932170000	H	6.247040000	-4.754040000	1.555780000
H	4.377820000	1.302870000	-4.881000000	H	5.981540000	-3.803050000	-1.726120000
H	-1.260040000	-0.722110000	7.554820000	H	5.072270000	-2.179460000	-4.155040000
H	-0.730160000	0.858060000	-8.248540000	H	3.944810000	-1.104130000	-6.790770000
H	1.914990000	0.941250000	-6.162720000	H	-4.788070000	1.968700000	5.389840000
Frame 19:				Frame 20:			
N	-1.138660000	0.638060000	0.265220000	N	-1.513830000	0.148010000	-0.093800000
H	-1.148670000	0.478060000	1.265220000	H	-1.353830000	-0.351990000	0.766200000
H	-1.738670000	-0.141940000	0.035220000	H	-1.963830000	-0.591990000	-0.613800000
C	-2.108660000	1.688060000	0.085220000	C	-2.753820000	0.828010000	0.196200000
H	-1.738670000	2.618060000	0.525220000	H	-2.513830000	1.588010000	0.946200000
C	-2.348660000	2.038060000	-1.384780000	C	-3.193830000	1.598010000	-1.043800000
H	-2.548660000	1.078060000	-1.874780000	H	-3.233820000	1.028010000	-1.973800000
H	-3.328670000	2.488060000	-1.504780000	H	-4.173830000	2.058010000	-0.883800000
C	-1.168660000	2.728060000	-2.014780000	C	-2.293820000	2.768010000	-1.353800000
N	0.171330000	2.378060000	-1.834780000	N	-0.933820000	2.588010000	-1.583800000
C	-1.308660000	3.748060000	-2.914780000	C	-2.683820000	4.078010000	-1.353800000
H	-2.108660000	4.298060000	-3.384780000	H	-3.663820000	4.538010000	-1.243800000
C	0.791340000	3.408060000	-2.404780000	C	-0.473820000	3.838010000	-1.653800000
H	1.841340000	3.658060000	-2.324780000	H	0.556170000	4.148010000	-1.773800000
N	-0.018660000	4.188060000	-3.144780000	N	-1.493830000	4.718010000	-1.643800000
H	0.141340000	5.018060000	-3.704780000	H	-1.383820000	5.688010000	-1.883800000
C	-3.388660000	1.248060000	0.775220000	C	-3.783830000	-0.231990000	0.566200000
O	-3.978660000	0.208060000	0.475220000	O	-3.863820000	-1.251990000	-0.103800000
N	-3.808660000	2.058060000	1.745220000	N	-4.433820000	-0.051990000	1.726200000
H	-3.128660000	2.778060000	1.945220000	H	-4.353830000	0.808010000	2.236200000
C	-5.118660000	2.058060000	2.365220000	C	-5.223820000	-1.101990000	2.336200000
H	-5.568660000	3.048060000	2.325220000	H	-6.183820000	-0.631990000	2.586200000
H	-5.818660000	1.408060000	1.845220000	H	-5.433820000	-1.991990000	1.746200000
C	-5.088660000	1.748060000	3.855220000	C	-4.723820000	-1.671990000	3.656200000
O	-6.138660000	1.828060000	4.495220000	O	-5.543820000	-1.911990000	4.536200000
N	-3.898670000	1.438060000	4.365220000	N	-3.453820000	-2.071990000	3.726200000
H	-3.088660000	1.628060000	3.785220000	H	-2.813820000	-1.781990000	2.996200000
C	-3.608660000	0.838060000	5.655220000	C	-2.843820000	-2.711990000	4.866200000
H	-4.488670000	0.378060000	6.085220000	H	-3.443830000	-3.591990000	5.126200000
C	-2.498660000	-0.211940000	5.535220000	C	-1.443830000	-3.191990000	4.476200000
H	-2.598660000	-0.821940000	6.435220000	H	-1.033830000	-3.831990000	5.256200000
H	-2.798660000	-0.911940000	4.745220000	H	-1.473820000	-3.881990000	3.636200000
C	-1.048660000	0.188060000	5.285220000	C	-0.433820000	-2.041990000	4.426200000
H	-0.838660000	1.088060000	5.855220000	H	-0.273820000	-1.701990000	5.446200000
H	-0.338660000	-0.521940000	5.725220000	H	0.536170000	-2.481990000	4.196200000
C	-0.748660000	0.528060000	3.835220000	C	-0.493830000	-1.031990000	3.286200000
O	-1.428660000	0.018060000	2.915220000	O	-1.213830000	-1.261990000	2.296200000
O	0.271340000	1.228060000	3.655220000	O	0.086180000	0.068010000	3.436200000
C	-3.198660000	1.948060000	6.605220000	C	-2.883820000	-1.991990000	6.206200000
O	-2.483290000	1.686650000	7.606960000	O	-2.405320000	-2.543290000	7.231220000
N	2.711340000	-0.291940000	-6.184780000	N	2.816180000	1.148010000	-6.393800000
H	1.771530000	-0.632000000	-6.218400000	H	1.987040000	0.590300000	-6.432380000
C	3.201340000	-0.361940000	-4.824780000	C	3.296180000	1.208010000	-5.023800000
H	4.261330000	-0.141940000	-4.754780000	H	4.176180000	1.838010000	-4.953800000
C	2.341340000	0.618060000	-4.034780000	C	2.146170000	1.678010000	-4.123800000
H	2.431340000	1.558060000	-4.584780000	H	1.656180000	2.478010000	-4.673800000
H	1.291340000	0.368060000	-3.874780000	H	1.386180000	0.898010000	-4.023800000
C	2.981340000	1.088060000	-2.754780000	C	2.516180000	2.168010000	-2.753800000
N	2.441340000	0.778060000	-1.514780000	N	1.806170000	1.888010000	-1.593800000
C	4.191340000	1.708060000	-2.604780000	C	3.596180000	2.968010000	-2.473800000

H	4.901340000	2.018060000	-3.364780000	H	4.336180000	3.378010000	-3.143800000
C	3.421330000	1.108060000	-0.664780000	C	2.666170000	2.298010000	-0.663800000
H	3.491340000	0.868060000	0.385220000	H	2.566180000	2.248010000	0.416200000
N	4.421330000	1.778060000	-1.244780000	N	3.626170000	3.128010000	-1.103800000
H	5.141340000	2.278060000	-0.734780000	H	4.256170000	3.638010000	-0.503800000
C	2.981340000	-1.791940000	-4.324780000	C	3.606180000	-0.261990000	-4.743800000
O	1.909540000	-2.096010000	-3.739660000	O	2.678890000	-1.051130000	-4.426060000
N	3.371340000	-4.421940000	-2.044780000	N	4.936180000	-2.781990000	-2.453800000
H	2.622180000	-4.950730000	-2.443720000	H	4.120920000	-3.085860000	-2.946780000
C	3.501340000	-4.751940000	-0.644780000	C	5.106180000	-3.121990000	-1.063800000
H	4.241340000	-4.121940000	-0.154780000	H	5.636180000	-2.281990000	-0.623800000
C	2.211340000	-4.511940000	0.125220000	C	3.696180000	-3.421990000	-0.533800000
H	1.381340000	-5.031940000	-0.354780000	H	3.106180000	-4.091990000	-1.153800000
H	2.221340000	-4.961940000	1.125220000	H	3.736170000	-4.141990000	0.286200000
C	1.791340000	-3.081940000	0.345220000	C	2.836180000	-2.211990000	-0.263800000
N	2.041340000	-2.491940000	1.575220000	N	2.776180000	-1.611990000	0.976200000
H	2.441340000	-2.941940000	2.385220000	H	3.296180000	-1.831990000	1.816200000
C	1.261330000	-2.101940000	-0.444780000	C	1.956180000	-1.531990000	-1.063800000
H	1.021340000	-2.181940000	-1.494780000	H	1.876170000	-1.801990000	-2.103800000
C	1.531340000	-1.251940000	1.525220000	C	1.856180000	-0.631990000	0.886200000
H	1.491340000	-0.691940000	2.445220000	H	1.686180000	0.008010000	1.736200000
N	1.101330000	-0.941940000	0.295220000	N	1.296180000	-0.551990000	-0.323800000
C	3.971340000	-6.201940000	-0.534780000	C	5.886180000	-4.421990000	-0.923800000
O	3.688990000	-7.025540000	-1.443370000	O	5.878800000	-5.264020000	-1.858960000
Cu	0.551340000	0.748060000	-0.714780000	Cu	0.066180000	1.008010000	-0.903800000
O	-1.368660000	-4.021940000	-1.004780000	O	-1.483820000	-2.831990000	0.296200000
H	-1.828670000	-3.261940000	-0.644780000	H	-1.313820000	-2.291990000	1.056200000
H	-2.048660000	-4.501940000	-1.484780000	H	-2.383820000	-3.141990000	0.416200000
O	2.371340000	1.088060000	5.075220000	O	3.506170000	1.438010000	2.486200000
H	2.581340000	2.018060000	5.175220000	H	3.036170000	2.248010000	2.306200000
H	1.561340000	1.068060000	4.565220000	H	3.146170000	1.128010000	3.316200000
O	-0.638660000	3.618060000	4.525220000	O	-0.293820000	4.498010000	1.796200000
H	-0.408660000	3.648060000	5.455220000	H	0.206180000	5.028010000	1.176200000
H	-0.428660000	3.728060000	4.265220000	H	-0.113820000	4.888010000	2.656200000
O	2.641340000	4.288060000	1.115220000	O	-0.843820000	-3.011990000	-3.473800000
H	3.171330000	4.688060000	0.435220000	H	-0.613820000	-2.771990000	-4.373800000
H	1.741340000	4.568060000	0.915220000	H	-1.553820000	-3.651990000	-3.563800000
O	1.201340000	1.938060000	1.115220000	O	-0.053820000	-4.521990000	-1.273800000
H	0.921330000	1.768060000	2.015220000	H	-0.463830000	-3.981990000	-0.603800000
H	1.781340000	2.698060000	1.185220000	H	-0.213830000	-4.051990000	-2.093800000
O	-2.458660000	-1.921940000	0.215220000	O	2.376170000	0.238010000	4.626200000
H	-2.158660000	-2.011940000	1.125220000	H	1.526180000	0.068010000	4.226200000
H	-3.388660000	-1.691940000	0.295220000	H	2.186180000	0.828010000	5.356200000
O	-1.988670000	-2.551940000	2.805220000	O	0.256170000	1.958010000	1.346200000
H	-2.728660000	-2.741940000	3.385220000	H	0.336180000	1.538010000	2.206200000
H	-1.828670000	-1.611940000	2.925220000	H	0.076170000	2.878010000	1.546200000
H	4.540490000	-6.516870000	0.314800000	O	0.266180000	-1.361990000	-5.613800000
H	4.223770000	-4.641120000	-2.519460000	H	0.276180000	-0.501990000	-6.013800000
H	3.290100000	-0.852690000	-6.776890000	H	1.066180000	-1.391990000	-5.083800000
H	3.738890000	-2.532950000	-4.472800000	O	-2.003820000	1.418010000	4.286200000
H	-3.517840000	2.953020000	6.423330000	H	-1.793820000	1.628010000	5.196200000
				H	-1.223820000	0.978010000	3.966200000
				O	-4.153820000	2.408010000	2.746200000
				H	-3.823820000	3.208010000	2.326200000
				H	-3.443830000	2.138010000	3.326200000
				O	-3.563820000	4.658010000	1.456200000
				H	-2.623830000	4.788010000	1.586200000
				H	-3.693830000	4.858010000	0.526200000
				H	6.440630000	-4.619660000	-0.030260000
				H	5.633460000	-2.242190000	-2.925400000
				H	4.611690000	-0.620240000	-4.817930000
				H	3.519610000	0.740170000	-6.975900000
				H	-3.318810000	-1.016960000	6.276860000

Mono-aqua Complex – Model 2

Frame 1:				Frame 2:			
N	0.283960000	-1.386730000	0.051400000	N	0.817300000	-0.586220000	-0.277840000
H	-0.286040000	-1.576730000	-0.758600000	H	0.427300000	-0.766220000	-1.197840000
H	-0.136040000	-1.966730000	0.771400000	H	0.977300000	-1.566220000	-0.057840000
C	1.373960000	-2.256730000	-0.338600000	C	2.177300000	-0.256220000	-0.657840000
H	1.663960000	-1.926730000	-1.338600000	H	2.167300000	0.463780000	-1.477840000
C	2.483960000	-2.056730000	0.691400000	C	3.067300000	0.263780000	0.462160000
H	2.193960000	-2.106730000	1.741400000	H	2.957300000	-0.186220000	1.442160000
H	3.223960000	-2.836730000	0.551400000	H	4.117300000	0.153780000	0.192160000
C	3.233960000	-0.776730000	0.431400000	C	2.757300000	1.733780000	0.592160000
N	2.623960000	0.473270000	0.321400000	N	1.567300000	2.103780000	1.212160000
C	4.583960000	-0.666730000	0.231400000	C	3.507300000	2.783780000	0.132160000
H	5.423960000	-1.346730000	0.261400000	H	4.477300000	2.793790000	-0.347840000
C	3.613960000	1.343270000	0.131400000	C	1.697290000	3.433780000	1.222160000
H	3.453960000	2.393270000	-0.028600000	H	0.977300000	4.153780000	1.582160000
N	4.793960000	0.703270000	0.191400000	N	2.807300000	3.873780000	0.612160000
H	5.673960000	1.153270000	-0.008600000	H	3.017290000	4.863780000	0.532160000
C	0.903960000	-3.706730000	-0.318600000	C	2.767290000	-1.526210000	-1.247840000
O	0.753960000	-4.236730000	0.771400000	O	2.597300000	-2.566220000	-0.617840000
N	0.643960000	-4.426730000	-1.408600000	N	3.247300000	-1.456210000	-2.487840000
H	0.743960000	-3.946730000	-2.288600000	H	3.507300000	-0.536220000	-2.797840000
C	-0.076040000	-5.686730000	-1.428600000	C	3.717300000	-2.616210000	-3.227840000
H	0.653960000	-6.456730000	-1.668600000	H	4.697290000	-2.446220000	-3.677840000
H	-0.516040000	-5.926730000	-0.458600000	H	3.977300000	-3.436220000	-2.547840000
C	-1.176040000	-5.706730000	-2.478600000	C	2.877290000	-3.096220000	-4.387840000
O	-1.976040000	-6.636730000	-2.438600000	O	3.347300000	-3.876220000	-5.217840000
N	-1.326040000	-4.636730000	-3.268600000	N	1.617300000	-2.656220000	-4.477840000
H	-0.776040000	-3.826730000	-3.018600000	H	1.307300000	-2.096220000	-3.707840000
C	-2.256040000	-4.386730000	-4.348600000	C	0.747300000	-2.686220000	-5.637840000
H	-3.246040000	-4.606730000	-3.948600000	H	0.637300000	-3.726220000	-5.957840000
C	-2.276040000	-2.886730000	-4.628600000	C	-0.672700000	-2.256220000	-5.257840000
H	-3.026040000	-2.616730000	-5.368600000	H	-1.292700000	-2.526210000	-6.117840000
H	-2.706040000	-2.366730000	-3.778600000	H	-1.012700000	-2.896220000	-4.437840000
C	-1.016040000	-2.046730000	-4.878600000	C	-0.842700000	-0.776210000	-4.937840000
H	-0.306040000	-2.516730000	-5.558600000	H	-0.392700000	-0.116210000	-5.677840000
H	-1.306040000	-1.106730000	-5.348600000	H	-1.902700000	-0.526210000	-5.027840000
C	-0.206040000	-1.646730000	-3.658600000	C	-0.332700000	-0.306220000	-3.577840000
O	-0.546040000	-2.026730000	-2.518600000	O	-0.412700000	-1.136220000	-2.647840000
O	0.693960000	-0.786730000	-3.768600000	O	0.377300000	0.723790000	-3.527840000
C	-2.106040000	-5.116730000	-5.668600000	C	1.277300000	-2.076220000	-6.927840000
O	-3.095503510	-5.237814430	-6.436630650	O	0.625215280	-2.200387890	-7.996922980
N	2.923960000	3.543270000	4.861400000	N	-0.432700000	2.323780000	6.692160000
H	3.611720000	2.936620000	4.462700000	H	0.459363900	2.016547720	6.360753410
C	1.913960000	3.843270000	3.871400000	C	-1.362700000	2.393780000	5.582160000
H	1.933960000	4.903270000	3.631400000	H	-2.002700000	3.263780000	5.692160000
C	2.293960000	3.103270000	2.591400000	C	-0.622700000	2.303780000	4.242160000
H	3.333960000	3.373270000	2.391400000	H	0.317300000	2.863780000	4.312160000
H	2.183960000	2.023270000	2.651400000	H	-0.262700000	1.283780000	4.082160000
C	1.443960000	3.463270000	1.401400000	C	-1.192700000	2.933780000	3.002160000
N	0.733960000	2.553270000	0.631400000	N	-1.112700000	2.393780000	1.722160000
C	1.353960000	4.703270000	0.831400000	C	-2.022700000	4.023780000	2.992160000
H	1.743960000	5.643270000	1.191400000	H	-2.402700000	4.623780000	3.802160000
C	0.083960000	3.313270000	-0.248600000	C	-1.712700000	3.263780000	0.912160000
H	-0.506040000	3.053270000	-1.108600000	H	-1.802700000	3.203780000	-0.157840000
N	0.363960000	4.623270000	-0.128600000	N	-2.262700000	4.243780000	1.652160000
H	0.163960000	5.293270000	-0.868600000	H	-2.852700000	5.003780000	1.342160000
C	0.623960000	3.333270000	4.511400000	C	-2.112700000	1.073780000	5.722160000
O	0.389570000	2.097710000	4.556260000	O	-1.475772020	-0.010882510	5.759584020

N	-2.836040000	2.903270000	4.321400000	N	-5.032700000	-0.996220000	3.882160000
H	-2.557840000	1.979850000	4.585770000	H	-5.005208350	-1.849183670	4.403405800
C	-4.146040000	2.853270000	3.691400000	C	-5.732700000	-1.216220000	2.632160000
H	-4.246040000	3.563270000	2.871400000	H	-6.072700000	-0.276210000	2.192160000
C	-4.306040000	1.483270000	3.041400000	C	-4.772700000	-0.206220000	1.732160000
H	-4.016040000	0.693270000	3.731400000	H	-4.352700000	-2.856220000	2.262160000
H	-5.326040000	1.213270000	2.771400000	H	-5.372700000	-2.416220000	0.922160000
C	-3.396040000	1.293270000	1.861400000	C	-3.652700000	-1.266220000	1.062160000
N	-3.726040000	1.163270000	0.521400000	N	-3.682700000	-0.936220000	-0.277840000
H	-4.656040000	1.283270000	0.151400000	H	-4.412700000	-1.186220000	-0.937840000
C	-2.086040000	0.923270000	1.961400000	C	-2.412700000	-0.876220000	1.502160000
H	-1.526040000	0.813270000	2.881400000	H	-1.942700000	-1.026210000	2.462160000
C	-2.596040000	0.793270000	-0.098600000	C	-2.592700000	-0.196220000	-0.517840000
H	-2.626040000	0.673270000	-1.168600000	H	-2.282700000	0.193780000	-1.477840000
N	-1.526040000	0.703270000	0.701400000	N	-1.772700000	-0.116210000	0.522160000
C	-5.246040000	3.023270000	4.721400000	C	-6.882700000	-2.176220000	2.922160000
O	-4.986470000	2.895500000	5.946090000	O	-6.677882790	-3.217208910	3.598889310
O	2.693960000	2.383270000	-3.108600000	Cu	-0.042700000	0.903780000	0.742160000
H	2.533960000	1.903270000	-3.918600000	O	4.077300000	2.313780000	4.412160000
H	3.643960000	2.453270000	-3.048600000	H	4.607300000	2.693780000	3.722160000
O	3.393960000	-1.296730000	-3.138600000	H	4.477300000	2.633790000	5.222160000
H	2.453960000	-1.296730000	-3.338600000	O	2.317300000	-4.106220000	1.602160000
H	3.583960000	-2.196730000	-2.888600000	H	3.067300000	-4.676220000	1.742160000
O	0.033960000	-2.496730000	3.891400000	H	2.387300000	-3.836220000	0.682160000
H	-0.756040000	-2.626730000	3.361400000	O	3.697290000	-1.666220000	3.352160000
H	0.213960000	-3.356730000	4.261400000	H	3.517290000	-2.496220000	2.902160000
O	-2.076040000	-2.586730000	2.131400000	H	4.547300000	-1.396220000	3.012160000
H	-2.496040000	-3.366730000	2.501400000	O	2.097300000	2.723790000	-4.067840000
H	-2.246040000	-2.646730000	1.191400000	H	1.417300000	2.053780000	-4.017840000
O	-2.486040000	-2.226730000	-0.998600000	H	2.087290000	3.003780000	-4.987840000
H	-1.746040000	-2.136730000	-1.598600000	O	-0.262700000	-2.786220000	1.352160000
H	-3.226040000	-1.836730000	-1.468600000	H	0.397300000	-3.416220000	1.642160000
O	4.703960000	-1.416730000	3.211400000	H	-0.722700000	-3.226220000	0.642160000
H	5.643960000	-1.606730000	3.181400000	O	-3.232700000	-1.746220000	-3.127840000
H	4.283960000	-2.236730000	2.941400000	H	-3.542700000	-2.246220000	-3.887840000
O	0.503960000	-0.116730000	2.701400000	H	-2.282700000	-1.876220000	-3.137840000
H	0.503960000	0.573270000	3.371400000	O	0.507300000	-0.266220000	2.492160000
H	0.163960000	-0.886730000	3.151400000	H	1.147300000	-0.046220000	3.172160000
O	2.013960000	0.773270000	-5.328600000	H	0.387300000	-1.216220000	2.562160000
H	1.353960000	1.413270000	-5.588600000	O	2.047300000	0.163780000	4.832160000
H	1.553960000	0.183270000	-4.728600000	H	2.657300000	0.863780000	4.592160000
O	4.183960000	0.923270000	4.521400000	H	2.537300000	-0.646220000	4.652160000
H	4.033960000	0.023270000	4.241400000	O	-0.402700000	-3.586220000	-1.247840000
H	5.133960000	1.013270000	4.531400000	H	-0.082700000	-4.136220000	-1.967840000
O	-4.426040000	-0.716730000	-2.158600000	H	-0.442700000	-2.706210000	-1.627840000
H	-4.736040000	0.193270000	-2.098600000	H	-5.510533420	-0.296373510	4.413093250
H	-5.216040000	-1.216730000	-2.378600000	H	-7.863292130	-1.964282800	2.550109340
O	0.563960000	4.173270000	-3.398600000	H	2.204310870	-1.541855150	-6.925591890
H	1.153960000	3.553270000	-2.958600000	H	-3.180627820	1.069665400	5.788592150
H	0.663960000	3.973270000	-4.328600000	H	-0.340428080	3.228845830	7.107300620
Cu	0.573960000	0.483270000	0.461400000				
H	-0.080260000	4.026640000	4.921520000				
H	3.360780000	4.391920000	5.159700000				
H	-2.170540000	3.280310000	3.677230000				
H	-6.242870000	3.251860000	4.406800000				
H	-1.158831740	-5.529062190	-5.947308940				
Frame 3:				Frame 4:			
N	0.907110000	-0.105880000	-0.239300000	N	1.050880000	-0.275880000	-0.083860000
H	0.727110000	-0.385880000	-1.189300000	H	0.920880000	-0.975880000	-0.793860000
H	1.207100000	-0.905880000	0.300700000	H	1.000880000	-0.905880000	0.706140000
C	2.237110000	0.444120000	-0.359300000	C	2.490880000	-0.095880000	-0.143860000
H	2.407110000	1.194120000	-1.139300000	H	2.840880000	0.054120000	-1.163860000
C	2.767110000	1.134120000	0.900700000	C	3.010880000	1.104120000	0.636140000
H	2.677100000	0.394120000	1.700700000	H	2.670880000	1.174120000	1.666140000
H	3.847110000	1.294120000	0.870700000	H	4.100880000	1.094120000	0.686140000
C	2.097110000	2.464120000	1.150700000	C	2.630880000	2.424120000	0.016140000
N	0.717100000	2.504120000	1.020700000	N	1.320880000	2.674120000	-0.373860000

C	2.547110000	3.754120000	1.190700000	C	3.420880000	3.484120000	-0.353860000
H	3.577100000	4.074120000	1.190700000	H	4.480880000	3.664120000	-0.243860000
C	0.417110000	3.794120000	1.110700000	C	1.400880000	3.824120000	-1.043860000
H	-0.602900000	4.124120000	0.980700000	H	0.610880000	4.264120000	-1.633860000
N	1.477110000	4.624120000	1.130700000	N	2.650880000	4.304120000	-1.143860000
H	1.437110000	5.634120000	1.010700000	H	2.970880000	5.174120000	-1.553860000
C	3.107100000	-0.775880000	-0.599300000	C	3.110880000	-1.415880000	0.296140000
O	3.007110000	-1.735880000	0.150700000	O	2.860880000	-1.835880000	1.426140000
N	3.677100000	-0.845880000	-1.809300000	N	3.910880000	-2.085880000	-0.533860000
H	3.587110000	-0.115880000	-2.489300000	H	4.180880000	-1.695880000	-1.423860000
C	4.487110000	-1.945880000	-2.299300000	C	4.240880000	-3.475880000	-0.273860000
H	5.517110000	-1.595880000	-2.339300000	H	5.320880000	-3.495880000	-0.163860000
H	4.527100000	-2.685880000	-1.499300000	H	3.910880000	-3.915880000	0.666140000
C	3.867110000	-2.605880000	-3.529300000	C	3.710880000	-4.355880000	-1.393860000
O	3.847110000	-3.835880000	-3.559300000	O	3.280880000	-5.495880000	-1.213860000
N	3.417110000	-1.765880000	-4.459300000	N	3.690880000	-3.805880000	-2.613860000
H	3.417110000	-0.775880000	-4.299300000	H	3.990880000	-2.845880000	-2.603860000
C	2.637100000	-2.115880000	-5.639300000	C	3.240880000	-4.435880000	-3.843860000
H	3.067100000	-3.075880000	-5.919300000	H	3.520880000	-5.495880000	-3.823860000
C	1.147100000	-2.315880000	-5.339300000	C	1.720880000	-4.335880000	-3.943860000
H	0.767110000	-2.935880000	-6.139300000	H	1.440880000	-4.965880000	-4.783860000
H	0.997100000	-3.105880000	-4.599300000	H	1.190880000	-4.745880000	-3.083860000
C	0.217100000	-1.195880000	-4.869300000	C	1.180880000	-2.915880000	-4.153860000
H	0.357100000	-0.285880000	-5.449300000	H	1.720880000	-2.445880000	-4.973860000
H	-0.842890000	-1.365880000	-5.019300000	H	0.190880000	-2.985880000	-4.613860000
C	0.287100000	-0.765880000	-3.419300000	C	1.080880000	-2.025880000	-2.923860000
O	0.077100000	-1.645880000	-2.559300000	O	0.540880000	-2.475880000	-1.893860000
O	0.617110000	0.414120000	-3.149300000	O	1.600880000	-0.895880000	-3.023860000
C	2.947110000	-1.225880000	-6.839300000	C	3.930880000	-4.165880000	-5.163860000
O	2.236280820	-1.296424950	-7.875309580	O	3.392966220	-4.531073520	-6.241288890
N	-0.922900000	1.674120000	6.720700000	N	-2.489120000	5.134120000	4.056140000
H	-0.164407710	1.026122790	6.651496920	H	-1.490211030	5.179847580	4.046660290
C	-1.672900000	1.674120000	5.480700000	C	-2.959120000	4.534120000	2.816140000
H	-2.532900000	2.334120000	5.480700000	H	-3.609120000	5.284120000	2.376140000
C	-0.882890000	2.134120000	4.250700000	C	-1.729120000	4.324120000	1.926140000
H	-0.342890000	3.024120000	4.580700000	H	-1.239120000	5.304120000	1.936140000
H	-0.072890000	1.424120000	4.080700000	H	-0.859120000	3.754120000	2.256140000
C	-1.732890000	2.404120000	3.050700000	C	-1.959120000	3.924120000	0.496140000
N	-1.962900000	1.504120000	2.010700000	N	-1.649120000	2.694120000	-0.073860000
C	-2.592890000	3.464120000	2.910700000	C	-2.469120000	4.714120000	-0.493860000
H	-2.892900000	4.294120000	3.540700000	H	-2.909120000	5.704120000	-0.503860000
C	-2.972890000	1.994120000	1.270700000	C	-2.169120000	2.694120000	-1.303860000
H	-3.312890000	1.724120000	0.290700000	H	-2.279120000	1.784120000	-1.873860000
N	-3.252890000	3.234120000	1.720700000	N	-2.549120000	3.944120000	-1.633860000
H	-3.782900000	3.944120000	1.230700000	H	-2.869120000	4.274120000	-2.523860000
C	-2.152890000	0.254120000	5.220700000	C	-3.639120000	3.234120000	3.206140000
O	-1.353467440	-0.608084350	4.772260710	O	-2.954776450	2.191175890	3.372007570
N	-4.762900000	-2.355880000	3.630700000	N	-5.549120000	0.314120000	2.716140000
H	-3.839832560	-2.727915080	3.728354500	H	-5.168153930	0.023183400	3.593762210
C	-5.302900000	-2.735880000	2.340700000	C	-5.849120000	-0.855880000	1.906140000
H	-5.852900000	-1.925880000	1.870700000	H	-6.249120000	-0.445880000	0.976140000
C	-4.212900000	-3.235880000	1.390700000	C	-4.639120000	-1.795880000	1.956140000
H	-3.572890000	-3.975880000	1.870700000	H	-4.269120000	-1.955880000	2.966140000
H	-4.682890000	-3.875880000	0.650700000	H	-4.869120000	-2.825880000	1.676140000
C	-3.312890000	-2.185880000	0.790700000	C	-3.499120000	-1.275880000	1.126140000
N	-3.292890000	-1.935880000	-0.569300000	N	-3.319120000	-1.685880000	-0.173860000
H	-3.912890000	-2.235880000	-1.299300000	H	-3.879120000	-2.355880000	-0.693860000
C	-2.232890000	-1.555880000	1.340700000	C	-2.539120000	-0.325880000	1.356140000
H	-1.982890000	-1.675880000	2.390700000	H	-2.379120000	0.274120000	2.246140000
C	-2.432890000	-0.915880000	-0.719300000	C	-2.299120000	-0.955880000	-0.663860000
H	-2.162890000	-0.505880000	-1.689300000	H	-2.039120000	-1.045880000	-1.703860000
N	-1.672900000	-0.725880000	0.370700000	N	-1.739120000	-0.145880000	0.236140000
C	-6.292890000	-3.875880000	2.520700000	C	-7.039120000	-1.555880000	2.536140000
O	-6.026949730	-4.821960710	3.306688310	O	-7.041927070	-1.805047060	3.769622250
Cu	-0.482890000	0.834120000	0.760700000	Cu	-0.169120000	1.284120000	-0.043860000
O	1.307110000	-2.745880000	3.310700000	O	-0.669120000	1.714120000	5.696140000
H	1.967100000	-3.275880000	2.860700000	H	-1.479120000	1.444120000	5.246140000

H	0.467100000	-3.105880000	3.020700000	H	-0.019120000	1.084120000	5.396140000
O	1.277100000	2.854120000	-2.969300000	O	-1.769120000	-0.815880000	4.596140000
H	1.007110000	1.954120000	-3.139300000	H	-1.659120000	-1.555880000	3.996140000
H	1.597110000	3.174120000	-3.809300000	H	-2.559120000	-1.025880000	5.096140000
O	3.537100000	1.014120000	-3.799300000	O	2.090880000	0.274120000	4.736140000
H	2.637100000	1.304120000	-3.619300000	H	2.260880000	1.164120000	4.416140000
H	4.077100000	1.724120000	-3.449300000	H	2.780880000	-0.255880000	4.336140000
O	-0.052900000	-4.375880000	1.610700000	O	-1.279120000	-2.895880000	2.976140000
H	0.227110000	-4.285880000	0.700700000	H	-0.879120000	-3.655880000	3.396140000
H	0.337110000	-5.195880000	1.900700000	H	-1.059120000	-2.985880000	2.046140000
O	1.167110000	-3.785880000	-0.819300000	O	3.540880000	0.424120000	-4.613860000
H	1.997100000	-3.375880000	-0.579300000	H	3.510880000	0.344120000	-5.563860000
H	0.727110000	-3.125880000	-1.349300000	H	2.740880000	-0.005880000	-4.303860000
O	1.717100000	0.684120000	6.700700000	O	3.960880000	-1.165880000	3.716140000
H	2.167110000	1.344120000	7.230700000	H	3.540880000	-1.565880000	2.966140000
H	2.277100000	0.554120000	5.940700000	H	4.280880000	-1.905880000	4.236140000
O	3.357100000	0.054120000	4.650700000	O	1.870880000	2.734120000	3.466140000
H	4.207100000	-0.355880000	4.810700000	H	2.540880000	3.404120000	3.376140000
H	2.757110000	-0.675880000	4.510700000	H	1.230880000	3.104120000	4.076140000
O	-1.772890000	-3.395880000	-3.099300000	O	-0.119120000	1.434120000	2.036140000
H	-1.142900000	-4.095880000	-3.289300000	H	-0.679120000	1.004120000	2.686140000
H	-1.222890000	-2.625880000	-2.959300000	H	0.600880000	1.794120000	2.546140000
O	0.227110000	-0.405880000	2.480700000	O	-0.079120000	-3.335880000	0.546140000
H	0.757110000	-1.195880000	2.550700000	H	0.160880000	-3.215880000	-0.373860000
H	-0.332890000	-0.425880000	3.260700000	H	0.460880000	-4.065880000	0.846140000
H	-7.215662900	-3.873649100	1.979049560	H	-7.875775320	-1.837570910	1.931525990
H	-4.729140920	-1.358670160	3.697279650	H	-6.388254810	0.834869300	2.873216230
H	-1.523559260	1.405040720	7.473564390	H	-2.864240710	6.057015050	4.143025990
H	-3.170224160	-0.011502800	5.419133220	H	-4.700304380	3.204618560	3.339995800
H	3.768912760	-0.541783850	-6.799895830	H	4.875993910	-3.664508870	-5.180792230
Frame 5:				Frame 6:			
N	0.838200000	-0.464590000	-0.092610000	N	1.066670000	0.219910000	-0.166230000
H	0.458200000	-1.334590000	-0.422610000	H	0.866670000	-0.750090000	-0.366230000
H	1.098200000	-0.774600000	0.827390000	H	1.716670000	0.099910000	0.603770000
C	2.048200000	-0.614600000	-0.872610000	C	2.066670000	0.519910000	-1.166230000
H	1.538200000	-0.954600000	-1.772610000	H	1.786670000	0.129910000	-2.146230000
C	2.748190000	0.745400000	-0.942610000	C	2.186660000	2.039910000	-1.296230000
H	2.918200000	1.005410000	0.107390000	H	2.256670000	2.449910000	-0.286230000
H	3.688200000	0.615410000	-1.472610000	H	3.086670000	2.249910000	-1.866230000
C	1.988200000	1.795400000	-1.692610000	C	0.956670000	2.659910000	-1.906230000
N	0.738200000	2.275410000	-1.312610000	N	-0.323330000	2.519910000	-1.396230000
C	2.348200000	2.435410000	-2.852610000	C	0.946670000	3.419910000	-3.046230000
H	3.238200000	2.245400000	-3.422610000	H	1.726670000	3.679910000	-3.756230000
C	0.398200000	3.165410000	-2.232610000	C	-1.073330000	3.069910000	-2.356230000
H	-0.481800000	3.795400000	-2.232610000	H	-2.143330000	3.199910000	-2.276230000
N	1.278200000	3.205410000	-3.252610000	N	-0.383330000	3.589910000	-3.386230000
H	1.158200000	3.835400000	-4.032610000	H	-0.793330000	4.029910000	-4.196230000
C	2.958200000	-1.754600000	-0.432610000	C	3.386670000	-0.110090000	-0.736230000
O	3.178200000	-1.844600000	0.777390000	O	3.936660000	0.119910000	0.333770000
N	3.608200000	-2.404590000	-1.392610000	N	3.916670000	-1.000090000	-1.586230000
H	3.388200000	-2.214590000	-2.362610000	H	3.486670000	-1.130090000	-2.486230000
C	4.408200000	-3.604590000	-1.262610000	C	4.996670000	-1.940090000	-1.336230000
H	5.278200000	-3.424590000	-1.882610000	H	5.786670000	-1.630090000	-2.016230000
H	4.578200000	-3.804590000	-0.202610000	H	5.456670000	-1.840090000	-0.356230000
C	3.678200000	-4.874590000	-1.682610000	C	4.746670000	-3.430090000	-1.546230000
O	4.338200000	-5.904590000	-1.622610000	O	5.686670000	-4.190090000	-1.776230000
N	2.348200000	-4.824600000	-1.822610000	N	3.476670000	-3.810090000	-1.426230000
H	1.818200000	-3.964590000	-1.892610000	H	2.696670000	-3.200090000	-1.246230000
C	1.528200000	-5.994590000	-2.042610000	C	2.906670000	-5.070090000	-1.856230000
H	1.888200000	-6.884590000	-1.522610000	H	3.386670000	-5.830090000	-1.246230000
C	0.038200000	-5.774600000	-1.782610000	C	1.396670000	-5.160090000	-1.636230000
H	-0.571800000	-6.634590000	-2.072610000	H	1.026660000	-6.180090000	-1.726230000
H	-0.121800000	-5.564590000	-0.722610000	H	1.146670000	-4.930090000	-0.606230000
C	-0.571800000	-4.604590000	-2.562610000	C	0.516670000	-4.220090000	-2.476230000
H	-0.271800000	-4.744590000	-3.602610000	H	0.796670000	-4.250090000	-3.526230000
H	-1.651800000	-4.544590000	-2.542610000	H	-0.503330000	-4.580090000	-2.316230000
C	-0.221800000	-3.184600000	-2.152610000	C	0.506670000	-2.760090000	-2.056230000

O	-0.091800000	-2.294590000	-3.012610000	O	0.326670000	-1.900090000	-2.936230000
O	0.148200000	-2.974590000	-0.972610000	O	0.876670000	-2.420090000	-0.906230000
C	1.648200000	-6.694590000	-3.392610000	C	3.336670000	-5.610090000	-3.216230000
O	0.968937270	-7.727329680	-3.628452030	O	3.382550090	-6.851967580	-3.414234150
N	-0.701800000	6.615410000	2.797390000	N	-2.733330000	5.529910000	3.443770000
H	0.235908410	6.268370640	2.813718860	H	-1.789654850	5.469813230	3.769139920
C	-1.561800000	5.655400000	2.127390000	C	-3.323330000	4.419910000	2.723770000
H	-2.301800000	6.235410000	1.577390000	H	-4.343330000	4.639910000	2.443770000
C	-0.871800000	4.845410000	1.027390000	C	-2.493330000	4.149910000	1.463770000
H	-0.241800000	5.485410000	0.417390000	H	-2.523330000	5.099910000	0.923770000
H	-0.201800000	4.105410000	1.467390000	H	-1.473340000	4.039910000	1.823770000
C	-1.771800000	4.045400000	0.127390000	C	-3.053330000	3.179910000	0.463770000
N	-1.731800000	2.655400000	-0.012610000	N	-2.563340000	1.889910000	0.283770000
C	-2.751800000	4.545400000	-0.692610000	C	-4.203330000	3.249910000	-0.276230000
H	-3.031800000	5.575410000	-0.852610000	H	-4.893330000	4.079910000	-0.396230000
C	-2.691800000	2.385400000	-0.902610000	C	-3.413330000	1.259910000	-0.536230000
H	-3.071800000	1.445410000	-1.272610000	H	-3.373330000	0.229910000	-0.866230000
N	-3.281800000	3.485410000	-1.392610000	N	-4.373330000	2.079910000	-0.986230000
H	-3.961800000	3.485410000	-2.132610000	H	-5.123330000	1.809910000	-1.596230000
C	-2.151800000	4.935410000	3.337390000	C	-3.373330000	3.249910000	3.693770000
O	-1.432670830	4.161990120	4.021674660	O	-2.372088000	2.499227290	3.826285980
N	-4.041800000	1.975400000	4.837390000	N	-4.073330000	-0.140090000	4.953770000
H	-3.133432020	2.070848350	5.244522930	H	-3.481801300	-0.048451450	5.754829410
C	-4.551800000	0.655400000	4.497390000	C	-4.173330000	-1.540090000	4.583770000
H	-5.101800000	0.695410000	3.557390000	H	-4.823330000	-1.680090000	3.713770000
C	-3.331800000	-0.254600000	4.307390000	C	-2.773330000	-2.080090000	4.283770000
H	-2.551800000	0.015400000	5.017390000	H	-2.073330000	-1.810090000	5.063770000
H	-3.551800000	-1.314590000	4.457390000	H	-2.873330000	-3.160090000	4.343770000
C	-2.861800000	-0.274600000	2.877390000	C	-2.133330000	-1.670090000	2.983770000
N	-3.171800000	-1.304590000	2.017390000	N	-2.253330000	-2.430090000	1.833770000
H	-3.791800000	-2.074600000	2.247390000	H	-2.653340000	-3.350090000	1.733770000
C	-1.941800000	0.505410000	2.227390000	C	-1.553330000	-0.500090000	2.583770000
H	-1.461800000	1.375410000	2.647390000	H	-1.323330000	0.359910000	3.193770000
C	-2.581800000	-1.044590000	0.847390000	C	-1.693330000	-1.720090000	0.833770000
H	-2.541800000	-1.584590000	-0.092610000	H	-1.543330000	-2.110090000	-0.166230000
N	-1.791800000	0.025410000	0.927390000	N	-1.253330000	-0.520090000	1.223770000
C	-5.421800000	0.125410000	5.627390000	C	-4.763330000	-2.340090000	5.733770000
O	-5.157012500	0.427318430	6.819996150	O	-4.514275300	-2.010572030	6.922450040
Cu	-0.431800000	1.085400000	-0.122610000	Cu	-0.693330000	1.089910000	-0.006230000
O	0.398200000	-1.654590000	2.647390000	O	1.246670000	4.309910000	1.073770000
H	1.328200000	-1.564590000	2.857390000	H	0.926670000	4.859910000	0.363770000
H	0.318200000	-2.544590000	2.307390000	H	2.096660000	4.689910000	1.303770000
O	4.188200000	3.345410000	3.457390000	O	1.376670000	-3.520090000	1.343770000
H	5.098200000	3.645410000	3.437390000	H	2.076670000	-2.890090000	1.493770000
H	3.898200000	3.395410000	2.547390000	H	1.106670000	-3.360090000	0.433770000
O	2.678200000	3.795400000	1.257390000	O	0.196670000	5.449910000	3.733770000
H	3.238200000	3.875410000	0.487390000	H	0.586670000	4.919910000	3.033770000
H	2.638200000	4.685410000	1.617390000	H	0.606670000	6.309910000	3.643770000
O	3.678200000	-1.574600000	3.527390000	O	2.606670000	-1.960090000	-4.116230000
H	3.838200000	-1.464590000	2.597390000	H	2.676670000	-1.230090000	-4.736230000
H	4.238200000	-2.304590000	3.787390000	H	1.716670000	-1.890090000	-3.766230000
O	-0.221800000	-4.174590000	1.427390000	O	1.196670000	-2.270090000	4.063770000
H	0.218200000	-3.814590000	0.657390000	H	1.126670000	-2.710090000	3.223770000
O	0.338200000	-4.894590000	1.717390000	H	2.056670000	-2.530090000	4.393770000
O	0.768200000	1.645410000	1.617390000	O	3.786670000	-2.310090000	1.703770000
H	1.388200000	2.315400000	1.327390000	H	4.576670000	-2.820090000	1.513770000
H	0.748200000	1.725400000	2.567390000	H	4.066670000	-1.400090000	1.643770000
O	-0.691800000	-0.904590000	-5.242610000	O	-0.363330000	-0.690090000	-5.286230000
H	-1.641800000	-0.844600000	-5.342610000	H	-0.233330000	-1.300090000	-4.556230000
H	-0.561800000	-1.444590000	-4.462610000	H	0.456670000	-0.720090000	-5.766230000
O	0.888200000	1.935410000	4.457390000	O	0.086670000	1.869910000	1.953770000
H	0.278200000	1.515400000	5.067390000	H	0.606670000	1.319910000	2.553770000
H	1.698200000	1.455410000	4.547390000	H	0.676670000	2.589910000	1.723770000
H	-6.258811620	-0.504037750	5.408056730	O	1.726670000	6.219910000	-1.146230000
H	2.309941290	-6.307478790	-4.139030380	H	2.656670000	6.349910000	-1.316230000
H	-3.176791940	5.088402750	3.603631890	H	1.306670000	6.309910000	-1.996230000
H	-0.726671200	7.485555950	2.305223920	O	1.806670000	0.319910000	3.333770000

H	-4.599741480	2.786937900	4.663874740	H	2.756670000	0.219910000	3.263770000
				H	1.496670000	-0.520090000	3.693770000
				H	3.599332910	-4.932985340	-4.002001900
				H	-4.259855040	3.064925090	4.263641860
				H	-3.269730690	6.356234990	3.615412980
				H	-4.983533980	0.213556120	5.169323080
				H	-5.390408720	-3.183408060	5.532556350
Frame 7:				Frame 8:			
N	1.266140000	0.083860000	-0.741400000	N	1.016830000	-0.811000000	0.356670000
H	1.226140000	-0.836140000	-0.311400000	H	0.266830000	-1.391000000	0.686670000
H	2.126140000	0.443860000	-0.351410000	H	1.696830000	-0.961000000	1.086670000
C	1.776140000	-0.486140000	-1.961400000	C	1.636830000	-1.731000000	-0.573330000
H	1.066140000	-1.176140000	-2.411400000	H	0.926830000	-2.211000000	-1.253330000
C	1.946140000	0.633860000	-3.001400000	C	2.786830000	-1.061000000	-1.323330000
H	2.606140000	1.423860000	-2.631400000	H	3.516830000	-0.641000000	-0.633340000
H	2.336140000	0.243860000	-3.941410000	H	3.316840000	-1.791000000	-1.933330000
C	0.626140000	1.153860000	-3.501400000	C	2.236830000	-0.101000000	-2.353330000
N	-0.353860000	1.743860000	-2.711400000	N	1.466830000	1.019000000	-2.073330000
C	0.146140000	1.013860000	-4.771400000	C	2.576830000	0.029000000	-3.673330000
H	0.606140000	0.543860000	-5.631400000	H	3.256830000	-0.601000000	-4.233330000
C	-1.373860000	1.963860000	-3.551400000	C	1.206830000	1.619000000	-3.233330000
H	-2.263860000	2.463860000	-3.201400000	H	0.546830000	2.469000000	-3.383340000
N	-1.133860000	1.543860000	-4.801400000	N	1.936830000	1.109000000	-4.233330000
H	-1.843860000	1.433860000	-5.501400000	H	1.906840000	1.239000000	-5.233330000
C	3.066140000	-1.246140000	-1.681400000	C	2.226840000	-2.781000000	0.346670000
O	4.016140000	-0.706140000	-1.111400000	O	2.856830000	-2.371000000	1.326670000
N	3.166140000	-2.546140000	-1.931400000	N	1.916830000	-4.061000000	0.126670000
H	2.306140000	-3.026140000	-2.181400000	H	1.346830000	-4.241000000	-0.683330000
C	4.226140000	-3.526140000	-1.771400000	C	2.236830000	-5.071000000	1.126670000
H	4.546140000	-3.896140000	-2.751400000	H	2.996830000	-5.801000000	0.856670000
H	5.066140000	-2.996140000	-1.331400000	H	2.556830000	-4.571000000	2.046670000
C	3.866140000	-4.626140000	-0.781410000	C	0.976840000	-5.821000000	1.546670000
O	4.526140000	-5.656140000	-0.911400000	O	1.086830000	-7.001000000	1.866660000
N	2.946140000	-4.396140000	0.158600000	N	-0.183160000	-5.181000000	1.526660000
H	2.476140000	-3.516140000	0.338600000	H	-0.143170000	-4.211000000	1.236670000
C	2.456140000	-5.396140000	1.078600000	C	-1.463170000	-5.751000000	1.916670000
H	3.406140000	-5.676140000	1.548600000	H	-1.263170000	-6.021000000	2.956660000
C	1.476140000	-4.796140000	2.078600000	C	-2.513170000	-4.661000000	2.086670000
H	1.136140000	-5.546140000	2.788600000	H	-3.463170000	-5.071000000	2.436670000
H	1.986140000	-3.996140000	2.628600000	H	-2.353170000	-3.961000000	2.916670000
C	0.166140000	-4.236140000	1.518600000	C	-2.733170000	-3.861000000	0.806670000
H	-0.343860000	-5.106140000	1.098600000	H	-2.433160000	-4.511000000	-0.023330000
H	-0.413860000	-3.826140000	2.338600000	H	-3.813170000	-3.761000000	0.686670000
C	0.356140000	-3.036140000	0.588600000	C	-1.953170000	-2.561000000	0.766670000
O	-0.453860000	-2.846140000	-0.341400000	O	-2.493170000	-1.521000000	0.306670000
O	1.406140000	-2.376140000	0.748600000	O	-0.833170000	-2.471000000	1.296670000
C	1.936140000	-6.726140000	0.548600000	C	-2.073170000	-6.961000000	1.236670000
O	1.703772030	-7.672969670	1.344269070	O	-3.004713940	-7.594748760	1.797168850
N	-0.393860000	6.983860000	-0.451400000	N	3.426830000	6.219000000	-1.413330000
H	0.534864740	6.766660870	-0.751891100	H	4.102492920	5.555883630	-1.091217760
C	-1.263860000	5.933860000	0.018600000	C	2.116830000	5.879000000	-0.873330000
H	-2.313860000	6.233860000	0.078600000	H	1.366830000	6.589000000	-1.213330000
C	-1.213860000	4.783860000	-0.971400000	C	1.626830000	4.539000000	-1.413330000
H	-1.453860000	5.153860000	-1.961400000	H	1.476840000	4.469000000	-2.493330000
H	-0.303860000	4.183860000	-1.121400000	H	2.366830000	3.759000000	-1.223340000
C	-2.253860000	3.703860000	-0.811400000	C	0.196830000	4.169000000	-1.153330000
N	-2.043860000	2.333860000	-0.641400000	N	-0.203170000	2.919000000	-0.703330000
C	-3.593860000	3.963860000	-0.761400000	C	-0.863170000	4.899000000	-1.643330000
H	-4.223860000	4.803860000	-1.001400000	H	-0.863170000	5.869000000	-2.113330000
C	-3.263860000	1.803860000	-0.521400000	C	-1.513170000	2.959000000	-0.923330000
H	-3.413860000	0.743860000	-0.371400000	H	-2.253170000	2.229000000	-0.613330000
N	-4.203860000	2.753860000	-0.481400000	N	-1.973170000	4.139000000	-1.363330000
H	-5.193860000	2.553860000	-0.551400000	H	-2.953170000	4.329000000	-1.523330000
C	-0.833860000	5.493860000	1.408600000	C	2.226840000	5.689000000	0.636670000
O	0.210634030	4.807735170	1.556368370	O	2.721472400	4.630110090	1.103212080
N	-1.213860000	3.453860000	4.768600000	N	0.846830000	5.099000000	3.966670000
H	-0.385262150	3.748549370	5.244608180	H	1.719882350	4.657772990	3.759068650

C	-1.723860000	2.243860000	5.388600000	C	-0.093160000	4.459000000	4.866660000
H	-2.773860000	2.083860000	5.158600000	H	-1.083170000	4.559000000	4.436670000
C	-0.903860000	1.023860000	4.988600000	C	0.296830000	2.979000000	4.856670000
H	0.096140000	1.233860000	5.368600000	H	1.376830000	2.889000000	4.956660000
H	-1.143860000	0.073860000	5.488600000	H	0.036830000	2.499000000	5.806670000
C	-0.893860000	0.683860000	3.528600000	C	-0.183160000	2.239000000	3.646670000
N	-1.493860000	-0.476140000	3.088600000	N	-1.203170000	1.309000000	3.666670000
H	-1.883860000	-1.186140000	3.688600000	H	-1.803170000	1.069000000	4.436670000
C	-0.413860000	1.273860000	2.378600000	C	0.196830000	2.249000000	2.326670000
H	0.116140000	2.203860000	2.268600000	H	0.956830000	2.849000000	1.836670000
C	-1.453860000	-0.466140000	1.738600000	C	-1.333170000	0.779000000	2.446670000
H	-1.853860000	-1.216140000	1.068600000	H	-1.973170000	-0.061000000	2.216670000
N	-0.803860000	0.583860000	1.238600000	N	-0.433160000	1.259000000	1.576670000
C	-1.563860000	2.413860000	6.898590000	C	0.036830000	5.039000000	6.266670000
O	-0.724165930	3.233021510	7.354066520	O	1.137699760	5.511046170	6.652453280
Cu	-0.433860000	1.183860000	-0.681400000	Cu	0.576830000	1.089000000	-0.193330000
O	5.816140000	0.253860000	0.868600000	O	0.076830000	-1.911000000	3.926670000
H	6.096140000	-0.336140000	1.568600000	H	0.716830000	-2.571000000	4.196670000
H	5.156140000	-0.246140000	0.398590000	H	-0.173170000	-2.171000000	3.046670000
O	-3.093860000	-3.356140000	0.098600000	O	2.286830000	-0.021000000	2.806670000
H	-3.223860000	-3.756140000	0.958600000	H	1.616830000	-0.111000000	3.486670000
H	-2.153860000	-3.176140000	0.058590000	H	3.076830000	-0.371000000	3.216670000
O	3.016140000	0.393860000	3.708600000	O	-4.103170000	1.919000000	1.066670000
H	3.806140000	0.513860000	4.248600000	H	-4.353170000	1.009000000	1.236670000
H	3.266140000	-0.246140000	3.048600000	H	-4.663170000	2.179000000	0.326670000
O	2.086140000	5.233860000	-1.301400000	O	-5.103170000	2.119000000	-1.443330000
H	2.316140000	5.623860000	-2.151400000	H	-4.303170000	1.909000000	-1.913330000
H	2.236140000	4.293860000	-1.421400000	H	-5.813170000	1.729000000	-1.953330000
O	3.686140000	-1.496140000	1.858600000	O	4.576830000	3.899000000	-2.293340000
H	4.246140000	-2.266140000	1.848600000	H	4.316840000	2.989000000	-2.463330000
H	2.816140000	-1.836140000	1.648590000	H	5.366830000	4.029000000	-2.823330000
O	3.316140000	1.433860000	1.058590000	O	5.496830000	-2.771000000	1.866660000
H	3.176140000	1.023860000	1.918600000	H	4.576830000	-2.531000000	1.766670000
H	4.226140000	1.243860000	0.848600000	H	5.786830000	-2.971000000	0.976670000
O	1.126140000	2.863860000	0.128600000	O	-4.023160000	-2.501000000	-1.743330000
H	1.986140000	2.563860000	0.418600000	H	-4.943170000	-2.241000000	-1.673330000
H	0.866140000	3.523860000	0.768600000	H	-3.593160000	-2.031000000	-1.033330000
O	0.816140000	-3.866140000	-2.561400000	O	2.596830000	1.769000000	0.376670000
H	0.126140000	-3.976140000	-3.211400000	H	3.076830000	2.599000000	0.316670000
H	0.356140000	-3.666140000	-1.741400000	H	2.946830000	1.359000000	1.176670000
H	-2.165793150	1.836388340	7.568741450	O	-4.893170000	-0.571000000	1.226670000
H	-1.905022280	4.174321990	4.825426240	H	-5.433160000	-0.371000000	0.456660000
H	-1.419294470	5.767538950	2.261399110	H	-4.113170000	-0.981000000	0.876670000
H	-0.719391770	7.929050640	-0.476771760	H	-1.711599840	-7.276092090	0.280174320
H	1.768440500	-6.855334570	-0.500249680	H	1.883403910	6.456124540	1.298841880
				H	3.686233200	7.134854700	-1.106866050
				H	0.621944390	5.981536720	3.553686460
				H	-0.807775990	5.045656950	6.923553860
Frame 9:				Frame 10:			
N	-0.266190000	-1.147620000	0.573490000	N	-0.189650000	-0.660350000	-1.228680000
H	-0.896190000	-0.717620000	1.233490000	H	-0.699650000	-1.270350000	-0.598690000
H	0.433810000	-1.517620000	1.193490000	H	0.290350000	-1.370350000	-1.768680000
C	-1.036190000	-2.327620000	0.243490000	C	-1.259650000	-0.370350000	-2.158680000
H	-2.096190000	-2.227620000	0.013490000	H	-2.069650000	0.269650000	-1.798680000
C	-0.376190000	-3.017620000	-0.956510000	C	-0.659650000	0.469650000	-3.278690000
H	0.623810000	-3.417620000	-0.756510000	H	0.290350000	-0.010350000	-3.518680000
H	-0.946190000	-3.887620000	-1.246510000	H	-1.229650000	0.429650000	-4.208680000
C	-0.406190000	-2.247620000	-2.246510000	C	-0.239650000	1.859650000	-2.878680000
N	0.133810000	-0.977620000	-2.436510000	N	0.380350000	2.099650000	-1.648690000
C	-0.856190000	-2.747620000	-3.436510000	C	-0.339650000	3.009650000	-3.608680000
H	-1.256190000	-3.727620000	-3.666510000	H	-0.869650000	3.029650000	-4.548680000
C	0.003810000	-0.787620000	-3.746510000	C	0.530350000	3.419650000	-1.698680000
H	0.303810000	0.112380000	-4.266510000	H	0.880350000	4.029650000	-0.878680000
N	-0.586190000	-1.797620000	-4.406510000	N	0.110350000	4.039650000	-2.808680000
H	-0.756190000	-1.857620000	-5.406510000	H	0.080350000	5.049650000	-2.888680000
C	-1.186190000	-3.167620000	1.503490000	C	-1.899650000	-1.640350000	-2.688690000
O	-0.206190000	-3.327620000	2.223490000	O	-1.239650000	-2.600350000	-3.098690000

N	-2.386190000	-3.727620000	1.703490000	N	-3.219650000	-1.740350000	-2.508690000
H	-3.196190000	-3.467620000	1.153490000	H	-3.709650000	-0.920350000	-2.178680000
C	-2.616190000	-4.437620000	2.933490000	C	-4.169650000	-2.750350000	-2.908680000
H	-2.956190000	-5.437620000	2.653490000	H	-4.779650000	-2.290350000	-3.688690000
H	-1.756190000	-4.487620000	3.603490000	H	-3.549650000	-3.550350000	-3.298680000
C	-3.726190000	-3.777620000	3.753490000	C	-4.959650000	-3.400350000	-1.768680000
O	-4.486190000	-4.347620000	4.533490000	O	-6.019650000	-3.950350000	-2.048680000
N	-3.676190000	-2.447620000	3.713490000	N	-4.429650000	-3.350350000	-0.548680000
H	-2.866190000	-2.037620000	3.273490000	H	-3.509650000	-2.930350000	-0.518680000
C	-4.596190000	-1.577620000	4.423490000	C	-5.019650000	-3.850350000	0.671310000
H	-4.506190000	-1.867620000	5.463490000	H	-5.239650000	-4.900350000	0.541320000
C	-4.146190000	-0.117620000	4.253490000	C	-3.879650000	-3.760350000	1.681320000
H	-4.706190000	0.552380000	4.903490000	H	-4.099650000	-4.400350000	2.531320000
H	-3.136190000	0.042380000	4.633490000	H	-3.099650000	-4.330350000	1.171310000
C	-4.266190000	0.442380000	2.833490000	C	-3.439650000	-2.380350000	2.161320000
H	-5.116190000	0.042380000	2.283490000	H	-4.289650000	-1.780350000	2.491310000
H	-4.406190000	1.512380000	2.983490000	H	-2.939650000	-2.430350000	3.131310000
C	-3.046190000	0.452380000	1.933490000	C	-2.789650000	-1.540350000	1.071320000
O	-3.076190000	0.982380000	0.803490000	O	-3.019650000	-0.310350000	1.001320000
O	-1.976190000	0.002380000	2.393490000	O	-1.899650000	-2.100350000	0.391320000
C	-6.056190000	-1.697620000	4.013490000	C	-6.359650000	-3.240350000	1.091320000
O	-6.953008770	-1.163196070	4.716112030	O	-6.936472800	-3.645893730	2.133615690
N	6.393810000	0.622380000	-3.116510000	N	6.660350000	2.489650000	-1.078690000
H	6.587149580	-0.130516100	-2.487409630	H	6.607405500	1.795816330	-1.796876410
C	5.253810000	1.482380000	-2.886510000	C	5.560350000	2.649650000	-0.138680000
H	5.113810000	2.152380000	-3.736510000	H	5.710350000	3.589650000	0.391320000
C	3.963810000	0.672380000	-2.746510000	C	4.150350000	2.509650000	-0.718680000
H	3.973810000	-0.047620000	-3.566510000	H	4.100350000	3.119650000	-1.618690000
H	4.003810000	0.132380000	-1.796510000	H	4.190350000	1.449650000	-0.958680000
C	2.663810000	1.422380000	-2.846510000	C	3.090350000	2.869650000	0.291320000
N	1.563810000	1.442380000	-1.986510000	N	2.030350000	2.049650000	0.651310000
C	2.473810000	2.242380000	-3.916510000	C	3.060350000	4.039650000	0.991310000
H	3.103810000	2.362380000	-4.786510000	H	3.740350000	4.869650000	0.851310000
C	0.763810000	2.372380000	-2.516510000	C	1.350350000	2.729650000	1.591320000
H	-0.006190000	2.762380000	-1.866510000	H	0.390350000	2.429650000	1.981320000
N	1.303810000	2.912380000	-3.616510000	N	1.930350000	3.929650000	1.771320000
H	0.933810000	3.692380000	-4.146510000	H	1.520350000	4.669650000	2.321320000
C	5.483810000	2.212380000	-1.576510000	C	5.780350000	1.489650000	0.821320000
O	5.324370680	1.609186640	-0.483666260	O	5.473614280	0.319399210	0.474914380
N	4.753810000	4.272380000	1.293490000	N	5.350350000	-0.620350000	3.791320000
H	4.808281450	3.284141030	1.436376660	H	5.516319520	-1.038350710	2.910199600
C	3.803810000	4.842380000	2.223490000	C	4.310350000	-1.120350000	4.661320000
H	3.033810000	5.432380000	1.733490000	H	3.690350000	-0.320350000	5.071320000
C	3.133810000	3.682380000	2.963490000	C	3.300350000	-1.990350000	3.921310000
H	3.863810000	2.982380000	3.373490000	H	3.880350000	-2.690350000	3.311310000
H	2.503810000	4.102380000	3.733490000	H	2.670350000	-2.630350000	4.541320000
C	2.243810000	2.842380000	2.073490000	C	2.340350000	-1.280350000	3.011310000
N	0.973810000	3.252380000	1.733490000	N	1.060350000	-0.910350000	3.401310000
H	0.563810000	4.072380000	2.153490000	H	0.600350000	-1.060350000	4.281320000
C	2.363810000	1.632380000	1.453490000	C	2.400350000	-0.980350000	1.681320000
H	3.283810000	1.082380000	1.383490000	H	3.230350000	-0.970350000	0.981320000
C	0.343810000	2.232380000	1.123490000	C	0.320350000	-0.700350000	2.301320000
H	-0.686190000	2.272380000	0.803490000	H	-0.699650000	-0.350350000	2.321320000
N	1.183810000	1.242380000	0.813490000	N	1.120350000	-0.640350000	1.231320000
C	4.603810000	5.602380000	3.263490000	C	4.910350000	-2.000350000	5.751320000
O	5.714815820	5.156890500	3.651788500	O	5.719403820	-2.914981760	5.447262080
Cu	0.633810000	0.062380000	-0.706510000	Cu	0.830350000	0.679650000	-0.288680000
O	2.113810000	-5.047620000	1.283490000	O	1.900350000	-4.770350000	0.681320000
H	1.423810000	-4.837620000	1.913490000	H	1.030350000	-4.620350000	0.311310000
H	1.653810000	-5.487620000	0.573490000	H	2.130350000	-5.660350000	0.411320000
O	2.243810000	-1.577620000	2.393490000	O	-4.759650000	0.079650000	-0.828690000
H	1.803810000	-2.357620000	2.723490000	H	-5.009650000	0.999650000	-0.788680000
H	2.943810000	-1.407620000	3.023490000	H	-4.149650000	-0.040350000	-0.098690000
O	1.183810000	-4.897620000	-3.096510000	O	4.960350000	-1.930350000	-1.958680000
H	0.573810000	-5.477620000	-3.556510000	H	4.490350000	-1.860350000	-2.788680000
H	0.963810000	-4.987620000	-2.166510000	H	4.530350000	-1.290350000	-1.388680000
O	-4.156190000	0.062380000	-2.656510000	O	-3.499650000	1.049650000	3.191320000

H	-3.526190000	0.732380000	-2.916510000	H	-3.719650000	1.939650000	2.931320000
H	-5.006190000	0.402380000	-2.946510000	H	-3.179650000	0.629650000	2.391320000
O	-0.086190000	-0.867620000	4.233490000	O	1.530350000	-2.240350000	-2.898690000
H	0.763810000	-0.807620000	3.783490000	H	1.860350000	-3.100350000	-2.638680000
H	-0.716190000	-0.587620000	3.573490000	H	0.810350000	-2.440350000	-3.498680000
O	3.003810000	-2.867620000	-2.596510000	O	2.520350000	0.019650000	-1.828690000
H	3.673810000	-3.487620000	-2.286510000	H	2.940350000	0.649650000	-2.408680000
H	2.323810000	-3.427620000	-2.966510000	H	2.190350000	-0.660350000	-2.408680000
O	-3.796190000	3.622380000	0.573490000	O	3.460350000	1.619650000	-3.678680000
H	-4.346190000	3.702380000	-0.206510000	H	3.180350000	1.599650000	-4.598690000
H	-3.306190000	2.812380000	0.443490000	H	4.420350000	1.619650000	-3.718680000
O	-5.446190000	-0.137620000	-0.186510000	O	-0.849650000	-4.400350000	-0.218680000
H	-4.706190000	0.132380000	0.353490000	H	-1.639650000	-4.810350000	-0.568680000
H	-5.096190000	-0.147620000	-1.076510000	H	-1.129650000	-3.530350000	0.071320000
O	5.263810000	-0.327620000	1.143490000	H	-6.805668240	-2.469212550	0.498601890
H	5.173810000	0.132380000	1.983490000	H	6.195857540	1.669036390	1.790894140
H	5.363810000	0.382380000	0.503490000	H	7.468916840	3.073574960	-1.006224090
O	6.733810000	-1.347620000	-1.226510000	H	5.873222440	0.190376110	4.054108910
H	6.563810000	-2.257620000	-1.436510000	H	4.643689530	-1.840509230	6.775157450
H	6.143810000	-1.147620000	-0.496510000				
O	-1.626190000	4.762380000	-0.566510000				
H	-2.386190000	4.642380000	0.013490000				
H	-1.956190000	4.542380000	-1.436510000				
O	2.473810000	-1.177620000	-0.586510000				
H	2.923810000	-1.497620000	0.193490000				
H	2.653810000	-1.827620000	-1.266510000				
O	-1.606190000	2.322380000	3.913490000				
H	-0.776190000	2.612380000	3.533490000				
H	-1.756190000	1.462380000	3.523490000				
H	4.223665090	6.517475000	3.667211420				
H	4.455941120	4.457868690	0.357077660				
H	5.781585580	3.240096400	-1.581867730				
H	6.988629050	0.780700290	-3.904624830				
H	-6.320578680	-2.236439360	3.127672680				
Frame 11:				Frame 12:			
N	-0.347330000	-0.973580000	-0.224410000	N	-0.441840000	-0.990620000	-0.493800000
H	-0.987330000	-0.943580000	0.555580000	H	-1.121840000	-0.730620000	0.206200000
H	0.102670000	-1.803580000	0.155580000	H	0.008160000	-1.810620000	-0.133800000
C	-1.337330000	-1.383590000	-1.194420000	C	-1.211840000	-1.570620000	-1.573800000
H	-2.077330000	-0.593580000	-1.114420000	H	-2.061840000	-0.980620000	-1.913800000
C	-0.777330000	-1.393580000	-2.624420000	C	-0.231840000	-1.890620000	-2.713800000
H	-0.017330000	-2.113580000	-2.884410000	H	0.648160000	-2.440620000	-2.373800000
H	-1.607330000	-1.693580000	-3.274420000	H	-0.791840000	-2.470620000	-3.443800000
C	-0.557330000	0.016420000	-3.114420000	C	0.088160000	-0.630620000	-3.463800000
N	0.282670000	0.876420000	-2.414420000	N	0.618160000	0.469380000	-2.793800000
C	-1.157330000	0.606420000	-4.194420000	C	-0.181840000	-0.300620000	-4.773800000
H	-1.837330000	0.106420000	-4.864420000	H	-0.551840000	-0.810620000	-5.643800000
C	0.172670000	1.986420000	-3.144420000	C	0.568160000	1.459380000	-3.683800000
H	0.622660000	2.896420000	-2.794410000	H	0.878160000	2.469380000	-3.473800000
N	-0.557330000	1.846420000	-4.264420000	N	0.088160000	1.049380000	-4.873800000
H	-0.817330000	2.616410000	-4.874420000	H	-0.121840000	1.639380000	-5.663800000
C	-1.897330000	-2.703590000	-0.684420000	C	-1.791840000	-2.880620000	-1.073800000
O	-1.107330000	-3.603580000	-0.414420000	O	-1.041840000	-3.720620000	-0.583800000
N	-3.217330000	-2.863580000	-0.544410000	N	-3.131840000	-2.930620000	-0.983800000
H	-3.757330000	-2.103580000	-0.944420000	H	-3.541840000	-2.100620000	-1.373800000
C	-3.917330000	-3.953590000	0.105580000	C	-4.031840000	-4.000620000	-0.613800000
H	-4.767330000	-4.293590000	-0.484420000	H	-4.621840000	-4.360620000	-1.453800000
H	-3.317330000	-4.793590000	0.445580000	H	-3.401840000	-4.820620000	-0.293800000
C	-4.617330000	-3.523580000	1.385580000	C	-4.971840000	-3.570620000	0.506200000
O	-5.097330000	-4.413580000	2.085580000	O	-5.901840000	-4.300620000	0.826200000
N	-4.607330000	-2.243580000	1.755580000	N	-4.711840000	-2.490620000	1.246200000
H	-4.077330000	-1.643580000	1.135580000	H	-3.911840000	-1.910620000	1.046200000
C	-5.227330000	-1.733580000	2.955590000	C	-5.461840000	-1.950620000	2.366200000
H	-5.607330000	-2.643580000	3.435580000	H	-5.511840000	-2.730620000	3.126200000
C	-4.247330000	-1.053580000	3.905580000	C	-4.551840000	-0.880620000	2.966200000
H	-4.737330000	-0.973580000	4.875580000	H	-5.021840000	-0.460620000	3.856200000
H	-3.467330000	-1.793590000	4.075580000	H	-3.601840000	-1.290620000	3.306200000

C	-3.617330000	0.286420000	3.505580000	C	-4.231840000	0.329380000	2.086200000
H	-4.407330000	1.016420000	3.315580000	H	-5.121840000	0.749380000	1.606200000
H	-2.997330000	0.746420000	4.275590000	H	-4.001840000	1.129380000	2.786200000
C	-2.787340000	0.316420000	2.235580000	C	-3.191840000	0.209380000	0.976200000
O	-2.637330000	1.396420000	1.635580000	O	-3.321840000	0.939380000	-0.033800000
O	-2.267330000	-0.743580000	1.815580000	O	-2.321840000	-0.650620000	1.196200000
C	-6.487330000	-0.913580000	2.715580000	C	-6.831840000	-1.430620000	1.986200000
O	-7.119107720	-0.430742910	3.690923950	O	-7.736280000	-1.345390000	2.857000000
N	5.952670000	2.016420000	-3.554420000	N	6.508160000	0.649380000	-3.133800000
H	5.802248750	1.040329770	-3.711331780	H	5.931150000	-0.039190000	-3.573030000
C	5.212660000	2.436420000	-2.384410000	C	5.738160000	1.349380000	-2.113800000
H	5.532670000	3.466420000	-2.264420000	H	6.068160000	2.349380000	-1.853800000
C	3.702670000	2.296410000	-2.604420000	C	4.268160000	1.399380000	-2.553800000
H	3.442670000	2.856420000	-3.504420000	H	4.228160000	1.909380000	-3.513800000
H	3.492670000	1.276420000	-2.924420000	H	3.918160000	0.369380000	-2.653800000
C	2.782670000	2.826420000	-1.544410000	C	3.428160000	2.309380000	-1.713800000
N	2.092670000	2.076420000	-0.594420000	N	2.328160000	1.919380000	-0.943800000
C	2.582670000	4.166420000	-1.344420000	C	3.618160000	3.659380000	-1.613800000
H	2.982670000	5.036420000	-1.844420000	H	4.348160000	4.299380000	-2.083800000
C	1.582670000	2.976420000	0.245580000	C	1.888160000	3.049380000	-0.393800000
H	0.932670000	2.756420000	1.075580000	H	1.028160000	3.219380000	0.246200000
N	1.712660000	4.206410000	-0.274420000	N	2.508160000	4.119380000	-0.923800000
H	1.252670000	5.036420000	0.095580000	H	2.248160000	5.069380000	-0.703800000
C	5.612670000	1.566420000	-1.204420000	C	5.868160000	0.509380000	-0.853800000
O	4.965561870	0.518143430	-0.947636310	O	5.231260000	-0.570900000	-0.749290000
N	6.182670000	0.486420000	2.265580000	N	5.398160000	-0.030620000	3.216200000
H	6.701828590	-0.351697450	2.098147950	H	5.570620000	-0.916270000	2.785160000
C	5.462660000	0.366410000	3.515580000	C	4.508160000	0.059380000	4.356200000
H	4.952670000	1.276420000	3.835580000	H	4.238160000	1.109380000	4.356200000
C	4.472670000	-0.803580000	3.515580000	C	3.278160000	-0.820620000	4.106200000
H	4.932670000	-1.703590000	3.115590000	H	3.508160000	-1.880620000	3.996200000
H	4.312670000	-1.173580000	4.535580000	H	2.658160000	-0.800620000	4.996200000
C	3.162670000	-0.483580000	2.855580000	C	2.328160000	-0.340620000	3.046200000
N	2.112670000	0.066420000	3.565580000	N	1.068160000	0.109380000	3.396200000
H	2.062670000	0.176420000	4.565580000	H	0.638160000	0.149380000	4.306200000
C	2.762670000	-0.443580000	1.545580000	C	2.428160000	-0.240620000	1.686200000
H	3.392670000	-0.833580000	0.765580000	H	3.288160000	-0.430620000	1.066200000
C	1.152670000	0.366410000	2.665580000	C	0.458160000	0.629380000	2.316200000
H	0.182670000	0.776420000	2.915580000	H	-0.461840000	1.199380000	2.266200000
N	1.532670000	0.186420000	1.395580000	N	1.258160000	0.399380000	1.276200000
C	6.492670000	-0.083580000	4.545580000	C	5.178160000	-0.370620000	5.666200000
O	7.267502990	-1.040071650	4.284183500	O	6.171980000	-1.142150000	5.640940000
Cu	0.892670000	0.466420000	-0.524420000	Cu	0.918160000	0.379380000	-0.793800000
O	1.702670000	0.106420000	-5.534420000	O	-0.761840000	-2.320620000	2.326200000
H	1.232670000	-0.523580000	-6.074420000	H	-1.391840000	-1.830620000	1.786200000
H	1.012670000	0.606420000	-5.094420000	H	-1.071840000	-3.220620000	2.296200000
O	-1.237330000	-2.453590000	3.605580000	O	-1.791840000	-4.780620000	1.896200000
H	-1.147330000	-2.003580000	4.445580000	H	-1.631840000	-5.710620000	1.756200000
H	-1.737330000	-1.833580000	3.065580000	H	-1.701840000	-4.390620000	1.026200000
O	4.642670000	0.016420000	-5.184420000	O	-3.131840000	4.809380000	0.146200000
H	4.772670000	-0.483580000	-5.984420000	H	-3.381840000	5.739380000	0.136200000
H	3.692670000	0.156420000	-5.144420000	H	-2.171840000	4.829380000	0.096200000
O	3.172670000	-4.023580000	1.095580000	O	-3.691840000	2.999380000	-1.653800000
H	2.412670000	-3.513580000	1.375580000	H	-3.531840000	2.379380000	-0.943800000
H	2.992670000	-4.913580000	1.375580000	H	-3.731840000	3.849380000	-1.213800000
O	-4.177330000	2.756420000	-0.454420000	O	1.138160000	-3.330620000	-5.013800000
H	-3.787340000	2.396420000	0.345580000	H	1.798160000	-3.800620000	-5.513800000
H	-4.857330000	3.346420000	-0.134410000	H	0.308160000	-3.690620000	-5.313800000
O	0.142670000	-4.903580000	-2.474410000	O	1.478160000	-2.950620000	0.446200000
H	0.242670000	-5.803580000	-2.154420000	H	1.628160000	-3.820620000	0.076200000
H	-0.457330000	-4.493580000	-1.844420000	H	1.178160000	-3.120620000	1.336200000
O	-4.707330000	-0.733580000	-1.724410000	O	2.458160000	-1.090620000	-1.303800000
H	-5.177330000	-0.963580000	-2.524420000	H	2.238160000	-1.860620000	-0.783800000
H	-4.457330000	0.186420000	-1.854420000	H	2.698160000	-1.450620000	-2.163800000
O	2.472670000	-3.263580000	-1.264420000	O	-4.631840000	-0.650620000	-1.753800000
H	1.882670000	-3.813580000	-1.784420000	H	-4.361840000	0.069380000	-1.183800000
H	2.722670000	-3.823580000	-0.524420000	H	-4.501840000	-0.310620000	-2.643800000

O	2.662670000	-0.633590000	-1.474410000	O	3.008160000	-1.340620000	-4.243800000
H	3.592670000	-0.453590000	-1.354420000	H	2.358160000	-2.020620000	-4.423800000
H	2.612670000	-1.583580000	-1.564420000	H	2.678160000	-0.560620000	-4.693800000
O	0.492670000	-2.983580000	1.765580000	H	4.800790000	-0.014750000	6.602070000
H	-0.007330000	-2.693580000	2.515580000	H	5.840110000	0.792930000	2.860680000
H	-0.097330000	-3.573580000	1.295580000	H	6.826190000	1.304270000	-3.819350000
O	-2.287340000	3.676420000	3.125580000	H	6.501230000	0.836570000	-0.055630000
H	-2.427330000	4.476420000	2.615590000	H	-7.031140000	-1.135550000	0.977180000
H	-2.467330000	2.966420000	2.505580000				
H	6.927834880	2.184443320	-3.410122990				
H	-6.835732130	-0.747790750	1.717567030				
H	6.444551030	1.845172850	-0.591908120				
H	6.556739990	0.413891650	5.490734480				
H	6.810604820	1.263061760	2.315833730				
Frame 13:				Frame 14:			
N	-0.448770000	-1.047540000	-0.210270000	N	0.092460000	-1.372990000	-0.001200000
H	-0.868770000	-1.007540000	0.709740000	H	-0.037540000	-1.192990000	0.988800000
H	-0.068770000	-1.977540000	-0.110260000	H	1.082460000	-1.572990000	0.058800000
C	-1.638770000	-1.527540000	-0.880260000	C	-0.657540000	-2.602990000	-0.051200000
H	-2.468770000	-0.907540000	-0.540260000	H	-1.617540000	-2.512990000	0.468800000
C	-1.528770000	-1.417540000	-2.410260000	C	-0.947540000	-3.092990000	-1.471200000
H	-0.728770000	-2.077540000	-2.730260000	H	-0.047540000	-3.072990000	-2.091200000
H	-2.408770000	-1.867540000	-2.860260000	H	-1.307540000	-4.102990000	-1.611200000
C	-1.328770000	-0.017540000	-2.930260000	C	-1.857540000	-2.172990000	-2.241200000
N	-0.278770000	0.832460000	-2.620270000	N	-1.717540000	-0.792990000	-2.201200000
C	-2.238770000	0.662460000	-3.700260000	C	-2.897540000	-2.532990000	-3.061200000
H	-3.188770000	0.272460000	-4.050260000	H	-3.327540000	-3.462990000	-3.391200000
C	-0.438770000	1.922460000	-3.380260000	C	-2.747540000	-0.372990000	-2.951200000
H	0.231230000	2.762450000	-3.460270000	H	-3.007540000	0.657010000	-3.131200000
N	-1.608770000	1.842460000	-4.040260000	N	-3.427540000	-1.352990000	-3.551200000
H	-1.968770000	2.542460000	-4.670260000	H	-4.177540000	-1.272990000	-4.221200000
C	-1.948770000	-2.947540000	-0.430260000	C	0.072460000	-3.682990000	0.748800000
O	-1.048770000	-3.727540000	-0.120270000	O	1.242460000	-3.902990000	0.428800000
N	-3.238770000	-3.287540000	-0.340260000	N	-0.507540000	-4.322990000	1.758800000
H	-3.968770000	-2.617540000	-0.550260000	H	-1.477540000	-4.092990000	1.938800000
C	-3.778770000	-4.477540000	0.289730000	C	0.052460000	-5.282990000	2.688800000
H	-4.598770000	-4.917540000	-0.270260000	H	-0.647540000	-6.092990000	2.918800000
H	-3.158770000	-5.357540000	0.449740000	H	1.002460000	-5.742990000	2.428800000
C	-4.448770000	-4.147550000	1.619740000	C	0.162460000	-4.692990000	4.088800000
O	-5.288770000	-4.927540000	2.059740000	O	1.242460000	-4.902990000	4.628800000
N	-4.158770000	-3.017540000	2.279740000	N	-0.807540000	-3.902990000	4.568800000
H	-3.478770000	-2.357540000	1.949740000	H	-1.617540000	-3.752990000	3.978800000
C	-4.728770000	-2.697540000	3.569740000	C	-0.747540000	-3.062990000	5.738800000
H	-4.558770000	-3.517540000	4.269740000	H	-0.177540000	-3.772990000	6.328800000
C	-3.688770000	-1.767540000	4.209740000	C	-0.027540000	-1.722990000	5.538800000
H	-4.048770000	-1.537540000	5.209740000	H	0.202460000	-1.452990000	6.568800000
H	-2.738770000	-2.297540000	4.279740000	H	0.932460000	-1.862990000	5.038800000
C	-3.518770000	-0.367540000	3.609740000	C	-0.817540000	-0.562990000	4.928800000
H	-4.468770000	0.152460000	3.489740000	H	-1.867540000	-0.512990000	5.188800000
H	-3.158770000	0.342460000	4.359740000	H	-0.377540000	0.397010000	5.178800000
C	-2.668770000	-0.277540000	2.349740000	C	-0.827540000	-0.592990000	3.398800000
O	-2.808770000	0.712460000	1.609740000	O	-1.907540000	-0.232990000	2.878800000
O	-1.858770000	-1.197540000	2.129730000	O	0.192460000	-0.892990000	2.738800000
C	-6.158770000	-2.167540000	3.579740000	C	-2.087540000	-2.992990000	6.458800000
O	-6.709841060	-1.864416340	4.669697470	O	-2.248760000	-2.186290000	7.411070000
N	5.401230000	1.792460000	-4.260260000	N	1.502460000	1.617010000	-6.521200000
H	5.330737260	0.795517770	-4.293978820	H	2.164730000	0.925240000	-6.233340000
C	4.741230000	2.282460000	-3.070260000	C	0.932460000	2.257010000	-5.351200000
H	4.911230000	3.352450000	-2.990260000	H	0.432460000	3.207010000	-5.551200000
C	3.261230000	1.882460000	-3.160260000	C	-0.047540000	1.307010000	-4.671200000
H	2.981230000	2.202460000	-4.160260000	H	-0.757540000	1.017010000	-5.431200000
H	3.051230000	0.812460000	-3.050260000	H	0.442460000	0.427010000	-4.251200000
C	2.391230000	2.682460000	-2.230260000	C	-0.797540000	2.067010000	-3.611200000
N	1.811230000	2.192450000	-1.070260000	N	-0.607540000	1.847010000	-2.241200000
C	2.171230000	4.032460000	-2.290260000	C	-1.847540000	2.937010000	-3.711200000
H	2.511230000	4.782460000	-2.990260000	H	-2.427540000	3.337010000	-4.521200000
C	1.441230000	3.292460000	-0.410260000	C	-1.447540000	2.627010000	-1.561200000

H	0.931230000	3.282460000	0.539730000	H	-1.527540000	2.697010000	-0.491200000
N	1.591230000	4.442450000	-1.100260000	N	-2.317540000	3.177010000	-2.431200000
H	1.161230000	5.322460000	-0.870270000	H	-3.147540000	3.697010000	-2.191200000
C	5.411230000	1.632460000	-1.870270000	C	2.202460000	2.487010000	-4.541200000
O	4.986199030	0.532159040	-1.431798750	O	2.629960000	1.587210000	-3.772330000
N	6.051230000	1.452460000	1.749740000	N	4.352460000	4.167010000	-1.831200000
H	6.087650740	0.579076310	1.264049750	H	5.301270000	4.037120000	-2.119100000
C	5.511230000	1.512450000	3.089740000	C	4.322460000	4.607010000	-0.451200000
H	4.981230000	2.432460000	3.329740000	H	3.482460000	5.267010000	-0.221200000
C	4.541230000	0.362460000	3.349740000	C	4.052460000	3.387010000	0.428800000
H	4.951230000	-0.637540000	3.229740000	H	4.892460000	2.687010000	0.398800000
H	4.351230000	0.422460000	4.419740000	H	4.082460000	3.787010000	1.438800000
C	3.221230000	0.392460000	2.639740000	C	2.722460000	2.707010000	0.238800000
N	2.081230000	0.942450000	3.199740000	N	1.842460000	2.677010000	1.298800000
H	2.131230000	1.312460000	4.139740000	H	1.942460000	3.267010000	2.118800000
C	2.851230000	0.182460000	1.339740000	C	2.332460000	1.717010000	-0.631200000
H	3.441230000	-0.077540000	0.469730000	H	2.772460000	1.337010000	-1.551200000
C	1.111230000	0.962460000	2.279740000	C	0.912460000	1.747010000	1.038800000
H	0.161230000	1.362460000	2.609740000	H	0.032460000	1.557010000	1.628800000
N	1.521230000	0.502460000	1.099740000	N	1.162460000	1.147010000	-0.131200000
C	6.591230000	1.382460000	4.159740000	C	5.622460000	5.267010000	-0.001200000
O	7.610242920	0.676708990	3.942717570	O	6.662620000	5.148980000	-0.699560000
Cu	0.601230000	0.532460000	-0.760260000	Cu	-0.257540000	0.137010000	-1.171200000
O	-3.318770000	2.802460000	3.219730000	O	2.582460000	-1.462990000	2.388800000
H	-3.198770000	2.062460000	2.629730000	H	2.902460000	-2.082990000	3.038800000
H	-4.058770000	3.282460000	2.849740000	H	1.652460000	-1.362990000	2.578800000
O	3.581230000	-2.777540000	-0.410260000	O	-4.517540000	-0.232990000	2.918800000
H	3.561230000	-3.697540000	-0.660260000	H	-3.567540000	-0.092990000	2.938800000
H	3.031230000	-2.717540000	0.369740000	H	-4.877540000	0.507010000	3.418800000
O	3.921230000	-0.467540000	-5.460270000	O	-2.777540000	2.337010000	3.508800000
H	3.891230000	-0.987550000	-6.260260000	H	-2.567540000	1.497010000	3.098800000
H	3.361230000	-0.937540000	-4.840260000	H	-3.557540000	2.157010000	4.028800000
O	2.101230000	-4.397550000	-2.820260000	O	2.572460000	-1.282990000	-6.421200000
H	1.601230000	-5.117540000	-2.430260000	H	2.282460000	-1.632990000	-7.261200000
H	2.951230000	-4.437540000	-2.390260000	H	2.232460000	-1.892990000	-5.771200000
O	1.461230000	-2.947540000	1.259740000	O	3.192460000	-2.582990000	-1.171200000
H	1.281230000	-2.467540000	2.069740000	H	2.872460000	-3.322990000	-1.681200000
H	0.781230000	-3.617540000	1.219730000	H	3.062460000	-2.832990000	-0.261200000
O	1.671230000	-1.777540000	-4.120270000	O	1.522460000	-0.762990000	-2.381200000
H	1.611230000	-2.717540000	-3.960270000	H	2.252460000	-1.282990000	-2.041200000
H	1.271230000	-1.647550000	-4.980260000	H	1.452460000	-1.042990000	-3.301200000
O	-4.378770000	1.632460000	-0.290260000	O	1.252460000	-2.952990000	-4.551200000
H	-4.488770000	2.572460000	-0.100260000	H	1.602460000	-3.602990000	-3.941200000
H	-3.918770000	1.292460000	0.479740000	H	0.412460000	-3.312990000	-4.821200000
O	2.061230000	-0.957540000	-1.500260000	H	5.649680000	5.830200000	0.908180000
H	2.751230000	-1.527540000	-1.160260000	H	3.919840000	4.857640000	-2.410740000
H	1.741230000	-1.417540000	-2.280270000	H	1.961140000	2.302910000	-7.086130000
O	-0.178770000	-2.397550000	3.959740000	H	2.730760000	3.413610000	-4.626180000
H	-0.538770000	-1.977540000	4.739740000	H	-2.892010000	-3.629720000	6.155010000
H	-0.668770000	-2.017540000	3.229740000				
H	6.244173060	2.110561410	-1.398544560				
H	6.365125400	2.057978550	-4.240121350				
H	6.388458510	2.284254670	1.308803930				
H	6.482129250	1.891394560	5.094610380				
H	-6.693486900	-2.053434960	2.659980310				
Frame 15:				Frame 16:			
N	-0.365210000	-1.271190000	0.304870000	N	-1.032390000	-1.180980000	0.371490000
H	0.094790000	-1.071190000	1.184870000	H	-0.532390000	-1.360980000	1.221490000
H	0.354790000	-1.951190000	0.084870000	H	-1.102400000	-2.110980000	-0.018510000
C	-1.425210000	-2.021190000	0.934870000	C	-2.362390000	-1.280980000	0.941490000
H	-1.985210000	-1.361190000	1.604870000	H	-2.562390000	-0.410980000	1.561490000
C	-2.375210000	-2.591190000	-0.115130000	C	-3.352400000	-1.300980000	-0.218510000
H	-1.855210000	-3.081190000	-0.945130000	H	-3.042390000	-2.110980000	-0.878510000
H	-2.965210000	-3.371190000	0.364870000	H	-4.342390000	-1.440980000	0.211490000
C	-3.215210000	-1.521190000	-0.735130000	C	-3.452390000	-0.020980000	-1.008510000
N	-2.725210000	-0.281190000	-1.165130000	N	-2.352400000	0.789020000	-1.298510000
C	-4.565210000	-1.511190000	-0.975130000	C	-4.602400000	0.509020000	-1.518510000

H	-5.285210000	-2.261190000	-0.675130000	H	-5.632390000	0.179020000	-1.458510000
C	-3.775210000	0.468810000	-1.495130000	C	-2.852400000	1.889020000	-1.868510000
H	-3.735210000	1.508810000	-1.805130000	H	-2.342390000	2.829020000	-2.038510000
N	-4.915210000	-0.231190000	-1.365130000	N	-4.182390000	1.749020000	-1.958510000
H	-5.885210000	-0.031190000	-1.545130000	H	-4.752390000	2.539020000	-2.198510000
C	-0.685210000	-3.111190000	1.684870000	C	-2.452390000	-2.540980000	1.791490000
O	0.044790000	-3.941190000	1.144870000	O	-2.122390000	-3.600980000	1.261490000
N	-1.055210000	-3.071190000	2.974870000	N	-2.842390000	-2.490980000	3.071490000
H	-1.805210000	-2.501190000	3.334870000	H	-2.892390000	-1.570980000	3.471490000
C	-0.525210000	-3.921190000	4.024870000	C	-2.862390000	-3.600980000	4.001490000
H	-1.355210000	-4.581190000	4.254870000	H	-3.902390000	-3.760980000	4.281490000
H	0.234790000	-4.551190000	3.554870000	H	-2.462390000	-4.530980000	3.571490000
C	0.104790000	-3.081190000	5.124870000	C	-2.022390000	-3.260980000	5.221490000
O	0.364790000	-3.681190000	6.174870000	O	-2.392390000	-3.630980000	6.331490000
N	0.474790000	-1.821190000	4.904870000	N	-0.952390000	-2.490980000	5.031490000
H	0.214790000	-1.371190000	4.034870000	H	-0.752390000	-2.150980000	4.101490000
C	1.434790000	-1.051190000	5.664870000	C	-0.002390000	-2.220980000	6.101490000
H	2.014790000	-1.801190000	6.204870000	H	0.187610000	-3.110980000	6.681490000
C	2.444790000	-0.281190000	4.814870000	C	1.257610000	-1.900980000	5.291490000
H	3.244790000	0.118810000	5.434870000	H	1.997610000	-2.040980000	6.081490000
H	2.944790000	-0.941190000	4.104870000	H	1.507610000	-2.660980000	4.551490000
C	1.914790000	0.968810000	4.104870000	C	1.447610000	-0.470980000	4.781490000
H	1.504790000	1.748810000	4.734870000	H	1.177610000	0.289020000	5.521490000
H	2.814790000	1.408810000	3.674870000	H	2.487600000	-0.220980000	4.571490000
C	0.834790000	0.718810000	3.064870000	C	0.697610000	-0.230980000	3.481490000
O	0.014790000	1.628810000	2.804870000	O	0.187610000	0.909020000	3.361490000
O	0.934790000	-0.331190000	2.384870000	O	0.387610000	-1.160980000	2.711490000
C	0.874790000	-0.081190000	6.704870000	C	-0.402390000	-1.140980000	7.091490000
O	1.652340000	0.675030000	7.342930000	O	0.341520000	-0.879700000	8.072250000
N	-0.845210000	-1.081190000	-6.585130000	N	0.287610000	0.849020000	-6.748510000
H	-1.296820000	-1.807390000	-6.066800000	H	-0.276260000	0.072400000	-6.467580000
C	-0.665210000	0.078810000	-5.735130000	C	0.857610000	1.479020000	-5.578510000
H	-0.905210000	1.018810000	-6.225130000	H	1.067610000	2.539020000	-5.748510000
C	-1.505210000	-0.131190000	-4.465130000	C	-0.132390000	1.369020000	-4.418510000
H	-2.525210000	-0.451190000	-4.715130000	H	-1.152390000	1.569020000	-4.748510000
H	-1.115210000	-0.831190000	-3.735130000	H	-0.182390000	0.389020000	-3.968510000
C	-1.625210000	1.158810000	-3.695130000	C	0.107610000	2.359020000	-3.308510000
N	-0.965210000	1.388810000	-2.495130000	N	0.177610000	1.959020000	-1.978510000
C	-2.265210000	2.288810000	-4.125130000	C	0.307610000	3.709020000	-3.358510000
H	-2.755210000	2.498810000	-5.065130000	H	0.197610000	4.379020000	-4.198510000
C	-1.185210000	2.678810000	-2.215130000	C	0.377610000	3.059020000	-1.248510000
H	-0.675210000	3.288810000	-1.485130000	H	0.667610000	3.079020000	-0.208510000
N	-1.955210000	3.228810000	-3.175130000	N	0.457610000	4.129020000	-2.048510000
H	-2.125210000	4.218810000	-3.325130000	H	0.487600000	5.109020000	-1.798510000
C	0.814790000	0.158810000	-5.425130000	C	2.067610000	0.619020000	-5.248510000
O	1.334600000	-0.659040000	-4.622340000	O	1.910320000	-0.511810000	-4.719310000
N	4.114790000	1.638810000	-4.215130000	N	5.027610000	-0.100980000	-3.138510000
H	4.717090000	0.840680000	-4.229670000	H	5.141710000	-1.033970000	-3.479830000
C	4.544790000	2.548810000	-3.175130000	C	5.627610000	0.009020000	-1.818510000
H	3.864790000	3.388810000	-3.015130000	H	5.547610000	1.009020000	-1.398510000
C	4.614790000	1.778810000	-1.855130000	C	4.967610000	-1.100980000	-1.008510000
H	5.224790000	0.888810000	-2.015130000	H	4.867610000	-2.060980000	-1.518510000
H	5.114790000	2.368810000	-1.095130000	H	5.527610000	-1.240980000	-0.078510000
C	3.254790000	1.438810000	-1.305130000	C	3.587610000	-0.720980000	-0.538510000
N	2.674790000	2.278810000	-0.375130000	N	3.527610000	0.079020000	0.591490000
H	3.014790000	3.138810000	0.034870000	H	4.277610000	0.499020000	1.131490000
C	2.354790000	0.448810000	-1.585130000	C	2.317610000	-0.840980000	-1.008510000
H	2.484790000	-0.411190000	-2.215130000	H	1.917610000	-1.250980000	-1.938510000
C	1.454790000	1.768810000	-0.145130000	C	2.237600000	0.379020000	0.791490000
H	0.714790000	2.288810000	0.434870000	H	1.797610000	0.969020000	1.581490000
N	1.164790000	0.698810000	-0.885130000	N	1.467610000	-0.130980000	-0.178510000
C	5.904790000	3.058810000	-3.635130000	C	7.087610000	-0.410980000	-1.908510000
O	6.679110000	2.298730000	-4.272520000	O	7.407870000	-1.437550000	-2.562080000
Cu	-0.745210000	0.018810000	-1.105130000	Cu	-0.432390000	0.279020000	-0.768510000
O	0.054790000	4.198810000	2.594870000	O	0.887610000	-3.280980000	-3.088510000
H	-0.525210000	4.498810000	3.294870000	H	1.357610000	-3.520980000	-2.298510000
H	0.094790000	3.248810000	2.714870000	H	1.577600000	-3.120980000	-3.738510000

O	-2.075210000	2.308810000	4.134870000	O	-1.302390000	-1.370980000	-6.178510000
H	-1.185210000	2.288810000	3.774870000	H	-1.792390000	-0.970980000	-5.458510000
H	-2.145210000	3.168810000	4.554870000	H	-1.962390000	-1.590980000	-6.828510000
O	2.494790000	-2.211190000	1.994870000	O	-3.142390000	-1.440980000	-4.208510000
H	2.444790000	-2.721190000	2.804870000	H	-4.092390000	-1.360980000	-4.178510000
H	1.904790000	-1.461190000	2.144870000	H	-2.972390000	-2.360980000	-3.998510000
O	-0.725210000	-3.411190000	-4.945130000	O	1.157610000	3.199020000	4.081490000
H	-1.575210000	-3.831190000	-4.795130000	H	0.487600000	3.649020000	4.591490000
H	-0.165210000	-3.761190000	-4.245130000	H	0.777610000	2.339020000	3.891490000
O	-3.345210000	-1.411190000	3.954870000	O	-0.762400000	-1.250980000	-2.518510000
H	-3.475210000	-0.661190000	3.374870000	H	-1.512400000	-1.200980000	-3.108510000
H	-4.115210000	-1.951190000	3.834870000	H	-0.212390000	-1.950980000	-2.878510000
O	0.594790000	-1.921190000	-2.215130000	O	-2.362390000	0.469020000	3.841490000
H	0.934790000	-1.611190000	-3.055130000	H	-1.442390000	0.699020000	3.731490000
H	1.074790000	-2.731190000	-2.045130000	H	-2.812390000	1.309020000	3.941490000
O	1.124790000	-4.611190000	-1.855130000	O	0.967610000	-3.460980000	1.621490000
H	1.714790000	-4.831190000	-1.145130000	H	0.797610000	-4.210980000	2.191490000
H	0.264790000	-4.911190000	-1.565130000	H	0.737600000	-2.700980000	2.151490000
H	6.201510000	4.063270000	-3.416220000	H	7.841790000	0.166600000	-1.416070000
H	4.153870000	2.102600000	-5.100500000	H	5.475350000	0.539370000	-3.762600000
H	-0.178390000	-0.045130000	6.890400000	H	3.052710000	0.975440000	-5.466290000
H	1.418620000	0.910750000	-5.888690000	H	1.022660000	0.528430000	-7.345940000
H	-1.409630000	-0.833140000	-7.372470000	H	-1.316750000	-0.602240000	6.955060000
Frame 17:				Frame 18:			
N	-0.379490000	-1.429580000	0.147200000	N	-1.428890000	-0.233400000	-0.016600000
H	-0.019490000	-1.049580000	1.017200000	H	-1.548890000	-0.333400000	0.983400000
H	0.330510000	-2.139580000	0.097200000	H	-1.678890000	-1.203400000	-0.146610000
C	-1.619490000	-1.889580000	0.737200000	C	-2.658890000	0.466600000	-0.306610000
H	-2.179490000	-1.039580000	1.127200000	H	-2.458890000	1.396600000	0.223390000
C	-2.629490000	-2.369580000	-0.302800000	C	-2.928890000	0.916600000	-1.746600000
H	-2.119490000	-2.979580000	-1.032800000	H	-2.948890000	-0.023400000	-2.306610000
H	-3.389490000	-2.989580000	0.177200000	H	-3.948890000	1.296600000	-1.726600000
C	-3.209490000	-1.299580000	-1.192800000	C	-1.948890000	1.966600000	-2.206600000
N	-2.449490000	-0.299580000	-1.802800000	N	-0.588890000	1.646600000	-2.246600000
C	-4.549490000	-1.089580000	-1.372800000	C	-2.198890000	3.196600000	-2.746600000
H	-5.359490000	-1.629580000	-0.902800000	H	-3.118890000	3.706600000	-3.016600000
C	-3.369490000	0.380420000	-2.492800000	C	-0.048890000	2.756600000	-2.756610000
H	-3.259490000	1.250420000	-3.122800000	H	0.971110000	3.066600000	-2.896610000
N	-4.619490000	-0.029580000	-2.252800000	N	-0.958890000	3.676600000	-3.116600000
H	-5.439490000	0.420420000	-2.642800000	H	-0.848890000	4.576600000	-3.556610000
C	-1.389490000	-3.019580000	1.727210000	C	-3.898890000	-0.263400000	0.183400000
O	-0.919490000	-4.069580000	1.297200000	O	-4.258890000	-1.373400000	-0.196600000
N	-1.639490000	-2.719580000	3.007200000	N	-4.548890000	0.356600000	1.173390000
H	-2.139490000	-1.889580000	3.297200000	H	-4.248890000	1.206600000	1.633400000
C	-1.319490000	-3.739580000	3.987200000	C	-5.698890000	-0.283400000	1.783400000
H	-2.229490000	-3.829580000	4.587200000	H	-6.558890000	0.306600000	1.473390000
H	-1.139490000	-4.739580000	3.597200000	H	-5.868890000	-1.293400000	1.403390000
C	-0.229490000	-3.279580000	4.947200000	C	-5.488890000	-0.303400000	3.293400000
O	0.690510000	-4.079580000	5.147200000	O	-6.558890000	-0.333400000	3.903390000
N	-0.419490000	-2.079580000	5.497200000	N	-4.288890000	-0.193400000	3.863400000
H	-1.339490000	-1.689580000	5.337200000	H	-3.618890000	-0.423400000	3.143400000
C	0.520510000	-1.379580000	6.337200000	C	-3.818890000	-0.063400000	5.233400000
H	1.010510000	-2.209580000	6.847200000	H	-4.128890000	-1.013400000	5.653390000
C	1.610510000	-0.599580000	5.607200000	C	-2.308890000	-0.063400000	5.473390000
H	2.310510000	-0.179580000	6.327200000	H	-2.238890000	-0.053400000	6.553400000
H	2.230510000	-1.339580000	5.107200000	H	-1.918890000	-1.063400000	5.283400000
C	1.140510000	0.390420000	4.537200000	C	-1.458890000	0.996600000	4.783400000
H	0.500510000	1.180420000	4.917200000	H	-1.938890000	1.976600000	4.813390000
H	2.050510000	0.870420000	4.177200000	H	-0.478890000	1.036600000	5.253400000
C	0.740510000	-0.119580000	3.157200000	C	-1.068890000	0.706600000	3.343400000
O	1.120510000	-1.249580000	2.767200000	O	-1.558890000	-0.273400000	2.743390000
O	-0.129490000	0.550420000	2.547200000	O	-0.298890000	1.566600000	2.853390000
C	-0.199490000	-0.629580000	7.447200000	C	-4.398890000	1.146600000	5.953400000
O	0.452040000	0.099810000	8.239080000	O	-4.420480000	1.179670000	7.211180000
N	-0.929490000	0.330420000	-7.422800000	N	3.131110000	-1.013400000	-6.216600000
H	-0.545110000	-0.588300000	-7.513390000	H	2.622600000	-1.874440000	-6.220640000
C	-0.339490000	0.990420000	-6.272790000	C	3.531110000	-0.693400000	-4.856600000

H	-0.219490000	2.060420000	-6.432790000	H	4.381110000	-0.023400000	-4.856600000
C	-1.069490000	0.720420000	-4.962800000	C	2.311110000	-0.053400000	-4.186610000
H	-2.139490000	0.630420000	-5.112790000	H	1.861110000	0.666600000	-4.856600000
H	-0.819490000	-0.259580000	-4.562800000	H	1.541110000	-0.793400000	-3.976600000
C	-0.869490000	1.760420000	-3.892800000	C	2.731110000	0.766600000	-2.966600000
N	-0.529490000	1.520420000	-2.562800000	N	2.111110000	0.636600000	-1.716600000
C	-1.039490000	3.110420000	-4.032800000	C	3.691110000	1.696600000	-2.966600000
H	-1.369490000	3.750420000	-4.832800000	H	4.271110000	2.186600000	-3.736610000
C	-0.309490000	2.690420000	-1.972800000	C	2.851110000	1.486600000	-1.006610000
H	-0.169490000	3.050420000	-0.962800000	H	2.611110000	1.706600000	0.033400000
N	-0.549490000	3.670420000	-2.862790000	N	3.821110000	2.136600000	-1.666610000
H	-0.699490000	4.650420000	-2.692800000	H	4.401110000	2.886600000	-1.306610000
C	1.030510000	0.340420000	-6.122800000	C	4.031110000	-1.933400000	-4.136600000
O	1.121690000	-0.902990000	-5.951970000	O	3.220970000	-2.671580000	-3.518270000
N	4.690510000	0.590420000	-4.252800000	N	5.021110000	-3.873400000	-1.456600000
H	4.504940000	-0.371170000	-4.455060000	H	4.642750000	-4.735690000	-1.793190000
C	5.410510000	0.950420000	-3.052800000	C	4.921110000	-3.833400000	-0.016600000
H	5.120510000	1.940420000	-2.692800000	H	5.311110000	-2.863400000	0.303400000
C	5.040510000	-0.099580000	-2.002800000	C	3.471110000	-3.953400000	0.443390000
H	5.130510000	-1.109580000	-2.392800000	H	2.901110000	-4.703400000	-0.116600000
H	5.700510000	-0.009580000	-1.142800000	H	3.581110000	-4.393400000	1.443390000
C	3.680510000	0.170420000	-1.422800000	C	2.761110000	-2.623400000	0.463400000
N	3.510510000	0.820420000	-0.212800000	N	2.901110000	-1.773400000	1.533400000
H	4.280510000	1.170420000	0.327200000	H	3.311110000	-2.153400000	2.373400000
C	2.410510000	-0.139580000	-1.812800000	C	1.831110000	-2.033400000	-0.346610000
H	2.010510000	-0.659580000	-2.672800000	H	1.521110000	-2.353400000	-1.326610000
C	2.190510000	0.880420000	0.067210000	C	1.851110000	-0.933400000	-1.553400000
H	1.860510000	1.520420000	0.877200000	H	1.521110000	-0.353400000	2.403390000
N	1.460510000	0.360420000	-0.922800000	N	1.201110000	-1.033400000	0.393400000
C	6.880510000	0.990420000	-3.472800000	C	5.721110000	-4.943400000	0.643400000
O	7.273290000	0.307690000	-4.454210000	O	5.765290000	-6.085600000	0.117090000
Cu	-0.499490000	-0.069580000	-1.232800000	Cu	0.281110000	0.236600000	-0.926600000
O	1.860510000	-3.129580000	0.847200000	O	-1.648890000	3.836600000	2.483400000
H	1.180510000	-3.779580000	1.027200000	H	-1.318890000	3.066600000	2.943390000
H	1.760510000	-2.479580000	1.537200000	H	-1.118890000	3.876600000	1.683400000
O	1.540510000	-3.909580000	-2.332800000	O	-0.088890000	-4.093400000	-3.686610000
H	2.040510000	-3.729580000	-1.532800000	H	-0.898890000	-4.443400000	-4.056610000
H	1.300510000	-4.829580000	-2.252800000	H	0.211110000	-4.763400000	-3.076610000
O	-2.919490000	-0.649580000	4.707200000	O	-3.178890000	-2.583400000	-3.136600000
H	-2.829490000	0.200420000	4.287200000	H	-2.738890000	-2.293400000	-2.336600000
H	-3.639490000	-1.079580000	4.247200000	H	-4.088890000	-2.313400000	-3.026610000
O	-0.149490000	-1.879580000	-2.722800000	O	-4.098890000	2.886600000	1.913400000
H	0.420510000	-2.639580000	-2.642800000	H	-3.228890000	3.276600000	2.043400000
H	-0.889490000	-2.189580000	-3.252800000	H	-4.298890000	3.066600000	0.993390000
O	-2.119490000	1.950420000	3.497200000	O	-1.008890000	-0.333400000	-4.716600000
H	-1.359490000	1.420420000	3.247200000	H	-1.798890000	0.186600000	-4.876600000
H	-1.739490000	2.770420000	3.827200000	H	-1.038890000	-1.023400000	-5.386600000
O	-2.359490000	-3.299580000	-4.182790000	O	-0.498890000	-1.483400000	-2.416610000
H	-3.089490000	-2.969580000	-4.702800000	H	-0.158890000	-2.353400000	-2.626600000
H	-2.749490000	-3.929580000	-3.582800000	H	-0.688890000	-1.093400000	-3.276610000
H	7.575010000	1.598930000	-2.932170000	O	-1.368890000	-2.803400000	2.993390000
H	4.377820000	1.302870000	-4.881000000	H	-1.338890000	-1.853400000	3.003400000
H	-1.260040000	-0.722110000	7.554820000	H	-1.968890000	-3.033400000	3.703400000
H	-0.730160000	0.858060000	-8.248540000	O	-1.278890000	-3.283400000	0.283400000
H	1.914990000	0.941250000	-6.162720000	H	-2.158890000	-3.573400000	0.063390000
				H	-1.308890000	-3.143400000	1.233400000
				O	1.801110000	1.796600000	4.443390000
				H	1.061110000	1.586600000	3.863400000
				H	1.561110000	2.636600000	4.833390000
				H	6.247040000	-4.754040000	1.555780000
				H	5.981540000	-3.803050000	-1.726120000
				H	5.072270000	-2.179460000	-4.155040000
				H	3.944810000	-1.104130000	-6.790770000
				H	-4.788070000	1.968700000	5.389840000
Frame 19:				Frame 20:			
N	-1.138660000	0.638060000	0.265220000	N	-1.513830000	0.148010000	-0.093800000
H	-1.148670000	0.478060000	1.265220000	H	-1.353830000	-0.351990000	0.766200000

H	-1.738670000	-0.141940000	0.035220000	H	-1.963830000	-0.591990000	-0.613800000
C	-2.108660000	1.688060000	0.085220000	C	-2.753820000	0.828010000	0.196200000
H	-1.738670000	2.618060000	0.525220000	H	-2.513830000	1.588010000	0.946200000
C	-2.348660000	2.038060000	-1.384780000	C	-3.193830000	1.598010000	-1.043800000
H	-2.548660000	1.078060000	-1.874780000	H	-3.233820000	1.028010000	-1.973800000
H	-3.328670000	2.488060000	-1.504780000	H	-4.173830000	2.058010000	-0.883800000
C	-1.168660000	2.728060000	-2.014780000	C	-2.293820000	2.768010000	-1.353800000
N	0.171330000	2.378060000	-1.834780000	N	-0.933820000	2.588010000	-1.583800000
C	-1.308660000	3.748060000	-2.914780000	C	-2.683820000	4.078010000	-1.353800000
H	-2.108660000	4.298060000	-3.384780000	H	-3.663820000	4.538010000	-1.243800000
C	0.791340000	3.408060000	-2.404780000	C	-0.473820000	3.838010000	-1.653800000
H	1.841340000	3.658060000	-2.324780000	H	0.556170000	4.148010000	-1.773800000
N	-0.018660000	4.188060000	-3.144780000	N	-1.493830000	4.718010000	-1.643800000
H	0.141340000	5.018060000	-3.704780000	H	-1.383820000	5.688010000	-1.883800000
C	-3.388660000	1.248060000	0.775220000	C	-3.783830000	-0.231990000	0.566200000
O	-3.978660000	0.208060000	0.475220000	O	-3.863820000	-1.251990000	-0.103800000
N	-3.808660000	2.058060000	1.745220000	N	-4.433820000	-0.051990000	1.726200000
H	-3.128660000	2.778060000	1.945220000	H	-4.353830000	0.808010000	2.236200000
C	-5.118660000	2.058060000	2.365220000	C	-5.223820000	-1.101990000	2.336200000
H	-5.568660000	3.048060000	2.325220000	H	-6.183820000	-0.631990000	2.586200000
H	-5.818660000	1.408060000	1.845220000	H	-5.433820000	-1.991990000	1.746200000
C	-5.088660000	1.748060000	3.855220000	C	-4.723820000	-1.671990000	3.656200000
O	-6.138660000	1.828060000	4.495220000	O	-5.543820000	-1.911990000	4.536200000
N	-3.898670000	1.438060000	4.365220000	N	-3.453820000	-2.071990000	3.726200000
H	-3.088660000	1.628060000	3.785220000	H	-2.813820000	-1.781990000	2.996200000
C	-3.608660000	0.838060000	5.655220000	C	-2.843820000	-2.711990000	4.866200000
H	-4.488670000	0.378060000	6.085220000	H	-3.443830000	-3.591990000	5.126200000
C	-2.498660000	-0.211940000	5.535220000	C	-1.443830000	-3.191990000	4.476200000
H	-2.598660000	-0.821940000	6.435220000	H	-1.033830000	-3.831990000	5.256200000
H	-2.798660000	-0.911940000	4.745220000	H	-1.473820000	-3.881990000	3.636200000
C	-1.048660000	0.188060000	5.285220000	C	-0.433820000	-2.041990000	4.426200000
H	-0.838660000	1.088060000	5.855220000	H	-0.273820000	-1.701990000	5.446200000
H	-0.338660000	-0.521940000	5.725220000	H	0.536170000	-2.481990000	4.196200000
C	-0.748660000	0.528060000	3.835220000	C	-0.493830000	-1.031990000	3.286200000
O	-1.428660000	0.018060000	2.915220000	O	-1.213830000	-1.261990000	2.296200000
O	0.271340000	1.228060000	3.655220000	O	0.086180000	0.068010000	3.436200000
C	-3.198660000	1.948060000	6.605220000	C	-2.883820000	-1.991990000	6.206200000
O	-2.483290000	1.686650000	7.606960000	O	-2.405320000	-2.543290000	7.231220000
N	2.711340000	-0.291940000	-6.184780000	N	2.816180000	1.148010000	-6.393800000
H	1.771530000	-0.632000000	-6.218400000	H	1.987040000	0.590300000	-6.432380000
C	3.201340000	-0.361940000	-4.824780000	C	3.296180000	1.208010000	-5.023800000
H	4.261330000	-0.141940000	-4.754780000	H	4.176180000	1.838010000	-4.953800000
C	2.341340000	0.618060000	-4.034780000	C	2.146170000	1.678010000	-4.123800000
H	2.431340000	1.558060000	-4.584780000	H	1.656180000	2.478010000	-4.673800000
H	1.291340000	0.368060000	-3.874780000	H	1.386180000	0.898010000	-4.023800000
C	2.981340000	1.088060000	-2.754780000	C	2.516180000	2.168010000	-2.753800000
N	2.441340000	0.778060000	-1.514780000	N	1.806170000	1.888010000	-1.593800000
C	4.191340000	1.708060000	-2.604780000	C	3.596180000	2.968010000	-2.473800000
H	4.901340000	2.018060000	-3.364780000	H	4.336180000	3.378010000	-3.143800000
C	3.421330000	1.108060000	-0.664780000	C	2.666170000	2.298010000	-0.663800000
H	3.491340000	0.868060000	0.385220000	H	2.566180000	2.248010000	0.416200000
N	4.421330000	1.778060000	-1.244780000	N	3.626170000	3.128010000	-1.103800000
H	5.141340000	2.278060000	-0.734780000	H	4.256170000	3.638010000	-0.503800000
C	2.981340000	-1.791940000	-4.324780000	C	3.606180000	-0.261990000	-4.743800000
O	1.909540000	-2.096010000	-3.739660000	O	2.678890000	-1.051130000	-4.426060000
N	3.371340000	-4.421940000	-2.044780000	N	4.936180000	-2.781990000	-2.453800000
H	2.622180000	-4.950730000	-2.443720000	H	4.120920000	-3.085860000	-2.946780000
C	3.501340000	-4.751940000	-0.644780000	C	5.106180000	-3.121990000	-1.063800000
H	4.241340000	-4.121940000	-0.154780000	H	5.636180000	-2.281990000	-0.623800000
C	2.211340000	-4.511940000	0.125220000	C	3.696180000	-3.421990000	-0.533800000
H	1.381340000	-5.031940000	-0.354780000	H	3.106180000	-4.091990000	-1.153800000
H	2.221340000	-4.961940000	1.125220000	H	3.736170000	-4.141990000	0.286200000
C	1.791340000	-3.081940000	0.345220000	C	2.836180000	-2.211990000	-0.263800000
N	2.041340000	-2.491940000	1.575220000	N	2.776180000	-1.611990000	0.976200000
H	2.441340000	-2.941940000	2.385220000	H	3.296180000	-1.831990000	1.816200000
C	1.261330000	-2.101940000	-0.444780000	C	1.956180000	-1.531990000	-1.063800000
H	1.021340000	-2.181940000	-1.494780000	H	1.876170000	-1.801990000	-2.103800000

C	1.531340000	-1.251940000	1.525220000	C	1.856180000	-0.631990000	0.886200000
H	1.491340000	-0.691940000	2.445220000	H	1.686180000	0.008010000	1.736200000
N	1.101330000	-0.941940000	0.295220000	N	1.296180000	-0.551990000	-0.323800000
C	3.971340000	-6.201940000	-0.534780000	C	5.886180000	-4.421990000	-0.923800000
O	3.688990000	-7.025540000	-1.443370000	O	5.878800000	-5.264020000	-1.858960000
Cu	0.551340000	0.748060000	-0.714780000	Cu	0.066180000	1.008010000	-0.903800000
O	-1.368660000	-4.021940000	-1.004780000	O	-1.483820000	-2.831990000	0.296200000
H	-1.828670000	-3.261940000	-0.644780000	H	-1.313820000	-2.291990000	1.056200000
H	-2.048660000	-4.501940000	-1.484780000	H	-2.383820000	-3.141990000	0.416200000
O	2.371340000	1.088060000	5.075220000	O	3.506170000	1.438010000	2.486200000
H	2.581340000	2.018060000	5.175220000	H	3.036170000	2.248010000	2.306200000
H	1.561340000	1.068060000	4.565220000	H	3.146170000	1.128010000	3.316200000
O	-0.638660000	3.618060000	4.525220000	O	-0.843820000	-3.011990000	-3.473800000
H	-0.408660000	3.648060000	5.455220000	H	-0.613820000	-2.771990000	-4.373800000
H	-0.428660000	2.728060000	4.265220000	H	-1.553820000	-3.651990000	-3.563800000
O	-0.148670000	0.198060000	-6.614780000	O	-0.053820000	-4.521990000	-1.273800000
H	-0.938660000	0.418060000	-6.114780000	H	-0.463830000	-3.981990000	-0.603800000
O	-0.228660000	0.698060000	-7.424780000	H	-0.213830000	-4.051990000	-2.093800000
H	-0.558660000	-0.501940000	-2.314780000	O	2.376170000	0.238010000	4.626200000
H	-1.268660000	0.018060000	-2.684780000	H	1.526180000	0.068010000	4.226200000
H	-0.618660000	-1.341940000	-2.764780000	H	2.186180000	0.828010000	5.356200000
O	-2.328670000	0.808060000	-4.444780000	O	-1.683820000	1.298010000	-4.503800000
H	-2.758660000	1.438060000	-5.024780000	H	-2.183820000	0.668010000	-5.013800000
H	-2.798660000	-0.011940000	-4.594780000	H	-2.073820000	2.148010000	-4.703800000
O	-3.188660000	-1.891940000	-4.324780000	O	0.266180000	-1.361990000	-5.613800000
H	-2.438660000	-2.291940000	-3.884780000	H	0.276180000	-0.501990000	-6.013800000
H	-3.948660000	-2.201940000	-3.814780000	H	1.066180000	-1.391990000	-5.083800000
O	-2.458660000	-1.921940000	0.215220000	O	-2.003820000	1.418010000	4.286200000
H	-2.158660000	-2.011940000	1.125220000	H	-1.793820000	1.628010000	5.196200000
H	-3.388660000	-1.691940000	0.295220000	H	-1.223820000	0.978010000	3.966200000
O	-1.988670000	-2.551940000	2.805220000	O	-4.153820000	2.408010000	2.746200000
H	-2.728660000	-2.741940000	3.385220000	H	-3.823820000	3.208010000	2.326200000
H	-1.828670000	-1.611940000	2.925220000	H	-3.443830000	2.138010000	3.326200000
O	-0.738670000	-2.851940000	-3.554780000	O	-0.483820000	-0.151990000	-2.723800000
H	0.021340000	-3.041940000	-4.104780000	H	-0.833830000	-1.011990000	-2.953800000
H	-0.608660000	-3.401940000	-2.774780000	H	-0.893820000	0.458010000	-3.333800000
H	4.540490000	-6.516870000	0.314800000	O	-3.563820000	4.658010000	1.456200000
H	4.223770000	-4.641120000	-2.519460000	H	-2.623830000	4.788010000	1.586200000
H	3.290100000	-0.852690000	-6.776890000	H	-3.693830000	4.858010000	0.526200000
H	3.738890000	-2.532950000	-4.472800000	H	6.440630000	-4.619660000	-0.030260000
H	-3.517840000	2.953020000	6.423330000	H	5.633460000	-2.242190000	-2.925400000
				H	4.611690000	-0.620240000	-4.817930000
				H	3.519610000	0.740170000	-6.975900000
				H	-3.318810000	-1.016960000	6.276860000

QM Part of the ONIOM optimized structure used for EPR parameters calculation			
N	-6.99622400	11.16138800	-1.83839000
H	-6.20772900	10.70534300	-1.37732000
H	-7.81203300	10.89166100	-1.28888400
C	-6.81162900	12.62263500	-1.72696300
H	-5.81046900	12.84469000	-2.08658100
C	-7.83445600	13.36884800	-2.60215100
H	-8.83862000	12.95776400	-2.45650400
H	-7.86164000	14.42302800	-2.31120700
C	-7.41583300	13.26307200	-4.03195100
N	-7.31084500	12.02373700	-4.65183500
C	-6.98193100	14.22838100	-4.90058500
H	-6.87999300	15.29516200	-4.78849300
C	-6.83054900	12.25631400	-5.86878300
H	-6.60151800	11.52193300	-6.61997600
N	-6.62975100	13.56929700	-6.05811300
H	-6.15453100	13.92820100	-6.88294100
C	-6.92533600	13.01422700	-0.25441200

O	-7.86096700	12.59847300	0.44694000
N	-5.93074500	13.78971700	0.20543800
H	-5.18110600	14.03522600	-0.43758600
C	-5.77875300	14.14649400	1.61069400
H	-6.11938700	15.16614000	1.80348700
H	-6.40193500	13.46559500	2.19839300
C	-4.31928400	14.08518300	2.10518900
O	-3.96011400	14.88786900	2.94668100
N	-3.54820000	13.14749000	1.47060600
H	-4.05348800	12.43272100	0.96331900
C	-2.15956000	12.72027600	1.72847500
H	-2.14056495	12.03734396	2.55196939
C	-1.61345600	12.02170200	0.46137100
H	-0.56526200	11.75914400	0.64127000
H	-2.15982500	11.08233300	0.32047600
C	-1.72086500	12.84216300	-0.84101800
H	-1.31941400	13.85077200	-0.72904900
H	-1.11553200	12.36035900	-1.61839800
C	-3.14395000	12.93685200	-1.38967200
O	-3.87122800	11.89373200	-1.37138300
O	-3.54891800	14.04913800	-1.83827900
C	-12.28334400	8.52019500	-7.91027400
O	-11.94257596	7.40539552	-8.38426750
N	-11.44514000	9.18835400	-7.07617300
H	-11.71182400	10.07942700	-6.63257700
C	-10.14912800	8.61419300	-6.78350200
H	-9.80369400	8.09284800	-7.67978600
C	-9.14630400	9.71334600	-6.44132900
H	-9.27390400	10.51001700	-7.17746800
H	-9.35889900	10.14701700	-5.46673500
C	-7.73998300	9.21056700	-6.48047500
N	-6.89115200	9.32982900	-5.40297200
C	-7.05173800	8.64363900	-7.52074300
H	-7.34982700	8.37645900	-8.51783300
C	-5.70863700	8.86976700	-5.78214200
H	-4.81809100	8.85658600	-5.17655100
N	-5.76730500	8.44828400	-7.06047200
H	-4.97509200	8.11054300	-7.59032300
C	-10.29502500	7.59265000	-5.64028200
O	-10.29821300	7.93601700	-4.44874500
N	-10.52322900	6.33903000	-6.04826200
H	-10.48942000	6.16190600	-7.04193300
C	-10.62425500	5.21110200	-5.13160000
H	-11.15738143	5.50488658	-4.25161884
C	-9.17326600	4.78002600	-4.75261700
O	-8.23141200	4.98454000	-5.50445500
N	-9.07129600	4.24590600	-3.50992300
H	-9.91488400	4.07759200	-2.99061300
C	-7.83734600	3.84841900	-2.85857900
H	-7.05125524	3.80921811	-3.58344079
C	-7.46298400	4.86691300	-1.75046200
H	-8.31355900	4.95204600	-1.07158400
H	-6.63492300	4.46514200	-1.15864100
C	-7.08444900	6.24902100	-2.20620700
N	-5.76695900	6.66582000	-2.26187000
H	-4.91714300	6.12879200	-2.11770700
C	-7.81701100	7.36858800	-2.51891300
H	-8.88536100	7.45022600	-2.62261200
C	-5.73733100	7.97067100	-2.57636000
H	-4.83681100	8.55127300	-2.67739800
N	-6.96713600	8.43912100	-2.74171300
Cu	-7.18007100	10.25911200	-3.64475100
O	-3.82750200	11.89433700	-5.87650400
H	-2.97240800	11.66328900	-6.29137200
H	-3.70943200	12.80250600	-5.45783300
O	-3.79892700	14.21881600	-4.63148100
H	-4.02070400	13.98886700	-3.70662300

H	-2.90391300	14.61108900	-4.52334100
O	-9.56343200	10.30992700	-0.39771100
H	-8.83483100	9.81232700	0.04801500
H	-9.37666000	11.22043200	-0.10283800
O	-7.25416400	9.87897700	0.95821100
H	-7.31420200	10.82569600	1.16457000
H	-6.31923200	9.75389000	0.69027100
O	-4.53365100	9.88137100	0.20571200
H	-4.11715200	10.55936500	-0.37735200
H	-3.85717000	9.19394400	0.33876300
O	-10.41458900	12.33070800	-4.35931200
H	-9.60936500	12.52496300	-4.86463600
H	-10.15647500	11.51147800	-3.86513600
O	-4.82083800	10.66453200	-3.61688000
H	-4.37650700	10.98513800	-4.43267400
H	-4.36306900	11.10155900	-2.86677500
O	-2.91541500	6.73712200	-2.26705600
H	-2.86086800	7.52238700	-2.83146600
H	-2.70394700	7.06676000	-1.37017400
O	-9.48788400	10.13802700	-3.11634300
H	-9.81330500	9.30750600	-3.53866300
H	-9.58531100	10.07292900	-2.13357900
O	-1.49076000	15.15351800	-3.36906000
H	-0.88900100	14.38978800	-3.45254700
H	-2.11887800	14.85927600	-2.66998000
O	-12.35034400	11.69131500	-6.14041700
H	-11.65981200	11.98330600	-5.49257400
H	-12.11831900	12.14792000	-6.96652900
O	-2.29126900	7.78163500	0.33060000
H	-1.34547100	7.99712600	0.26716800
H	-2.30176100	7.03458300	0.95285900
O	-5.00847700	12.84836700	-8.20031000
H	-4.56570800	12.40114400	-7.44120300
H	-4.26949200	12.90963700	-8.83528500
H	-1.55692913	13.57466934	1.95595700
H	-13.23343053	8.94171853	-8.16434780
H	-11.13126573	4.39902219	-5.60947708
H	-7.96404051	2.88016715	-2.42115833

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