

Supporting information for

Density Functional Theory Investigations on the Binding Modes of Amidoximes with Uranyl Ions

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Table S1. The Wiberg bond order of U-O(AO1/TAO1/EtOH) of the species in Figure 4.^a

U-EtOH	0.4022		U-M2-EtOH	0.4738	0.3726
	U-O (EtOH)			U-N	U-O (EtOH)
U-EtOH-EtOH	0.3690		U-M1-EtOH	0.3673	0.3754
	U-O(EtOH)			U-O	U-O (EtOH)
U-M5	0.3129	0.3219	U-M6-EtOH	0.6563	0.3547
	U-O	U-N		U-O	U-O (EtOH)
U-M2	0.4584		U-M2-M2	0.4699	
	U-N			U-N	
U-M4	0.4118	0.2687	U-M6-M6	0.6394	0.5959
	U-N	U-O		U-N	U-N
U-M6	0.6402				
	U-O				

^aThe U-O and U-N distances correspond to the U-oxime bond lengths unless otherwise noted.

1. The relative enthalpies of the examined U-AO complexes

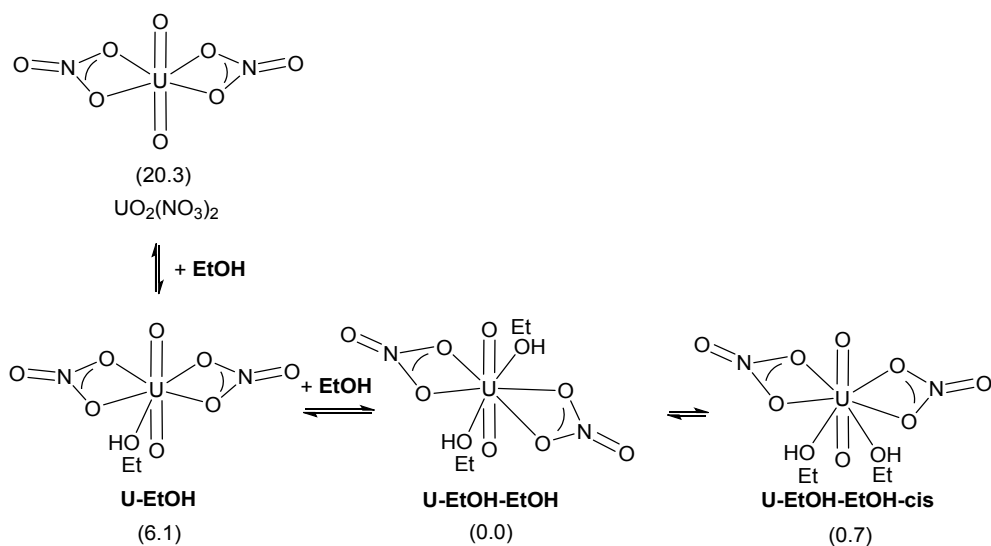


Figure S1. The equilibrium between the $\text{U}(\text{NO}_3)_2(\text{EtOH})_n$ ($n=0, 1, \text{ or } 2$) complexes.

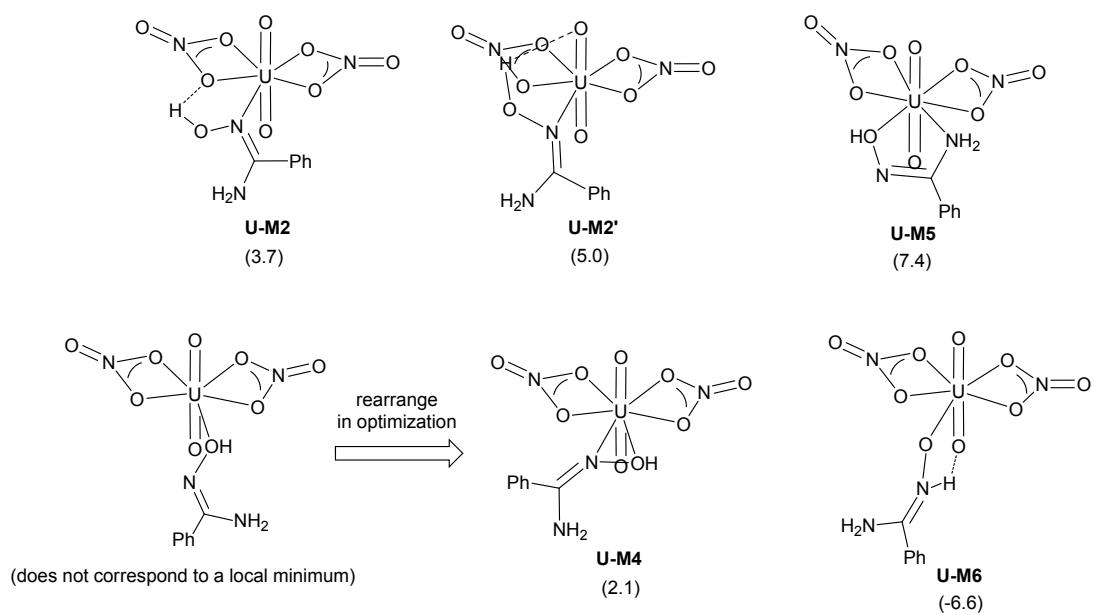


Figure S2. The comparison between the different $\text{UO}_2(\text{NO}_3)_2(\text{AO1})$ and $\text{UO}_2(\text{NO}_3)_2(\text{TAO1})$ complexes.

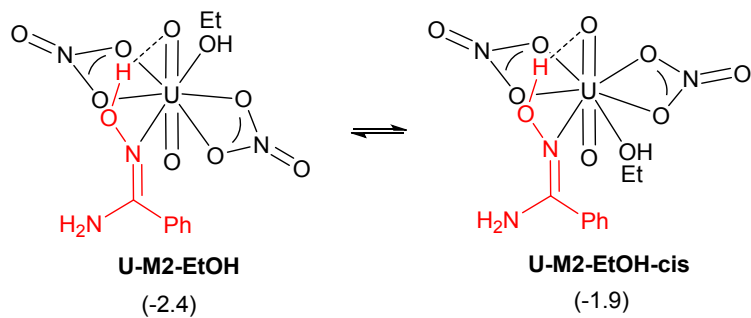


Figure S3. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{EtOH})(\text{AO1})$ via the $\eta^1\text{-N}$ coordination mode.

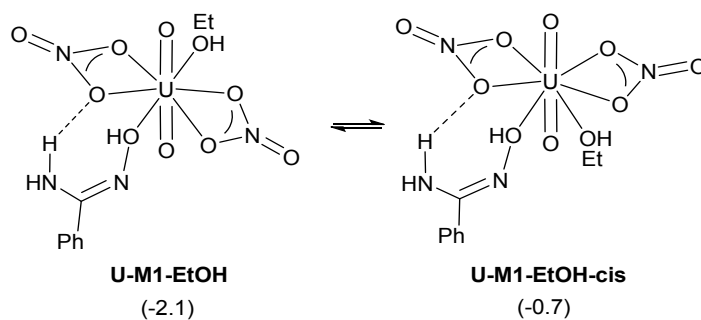


Figure S4. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{EtOH})(\text{AO1})$ via the $\eta^1\text{-O(H)}$ coordination mode.

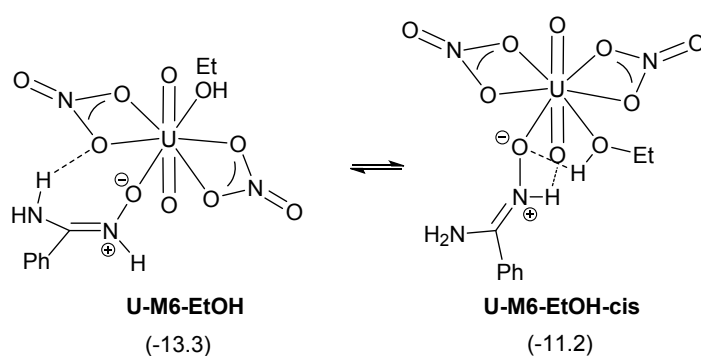


Figure S5. The comparison between $\text{UO}_2(\text{NO}_3)_2(\text{EtOH})(\text{TAO1})$ via the $\eta^1\text{-O}$ coordinated TAO1.

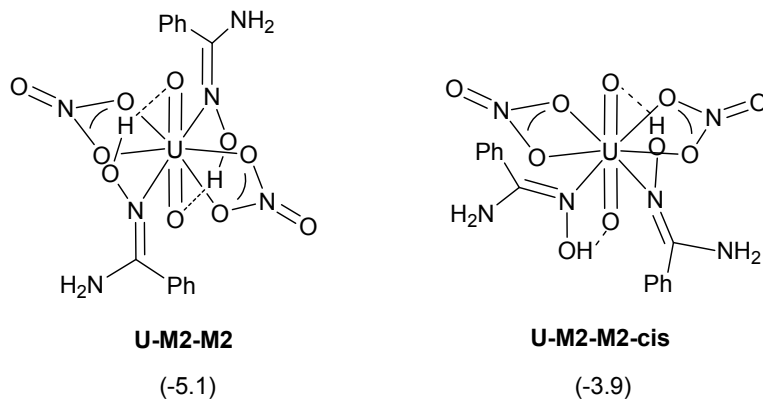


Figure S6. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AO1})_2$ with double $\eta^1\text{-N}$ coordination modes.

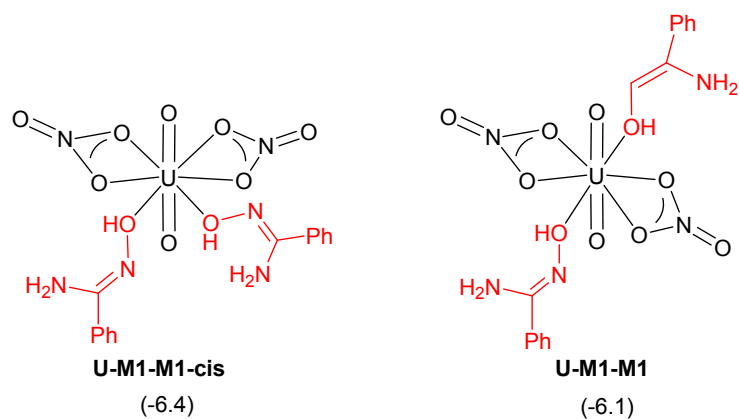


Figure S7. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AO1})_2$ with double $\eta^1\text{-O(H)}$ coordination modes.

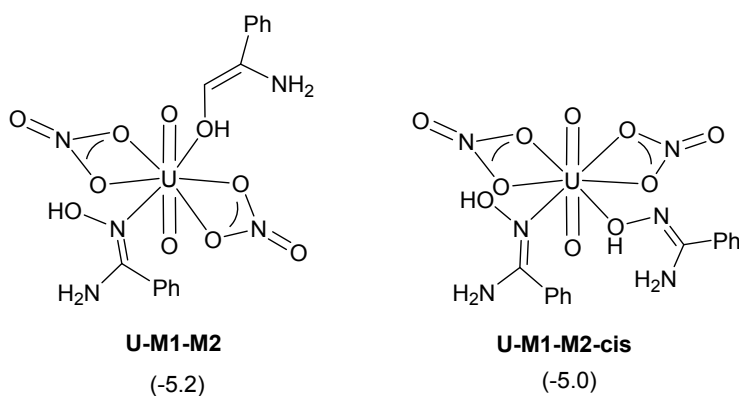


Figure S8. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AO1})_2$ with one $\eta^1\text{-O(H)}$ and another $\eta^1\text{-N}$ coordination modes.

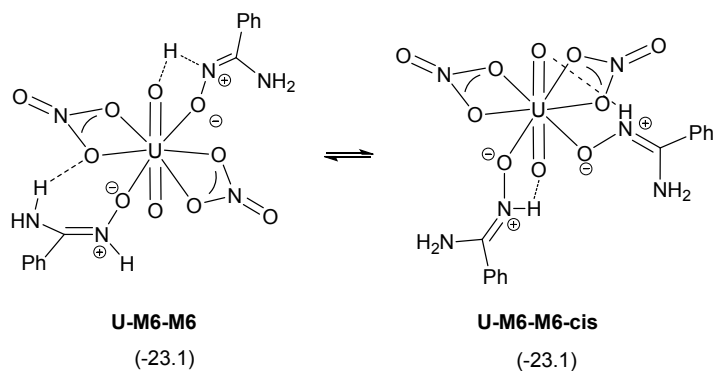


Figure S9. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{TAO1})_2$ with double $\eta^1\text{-O}$ modes.

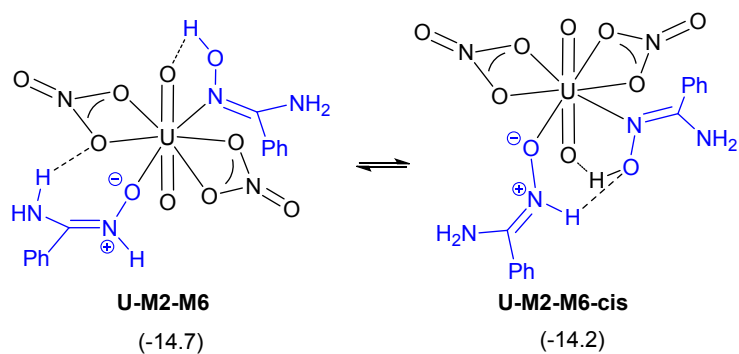


Figure S10. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{TAO1})(\text{AO1})$.

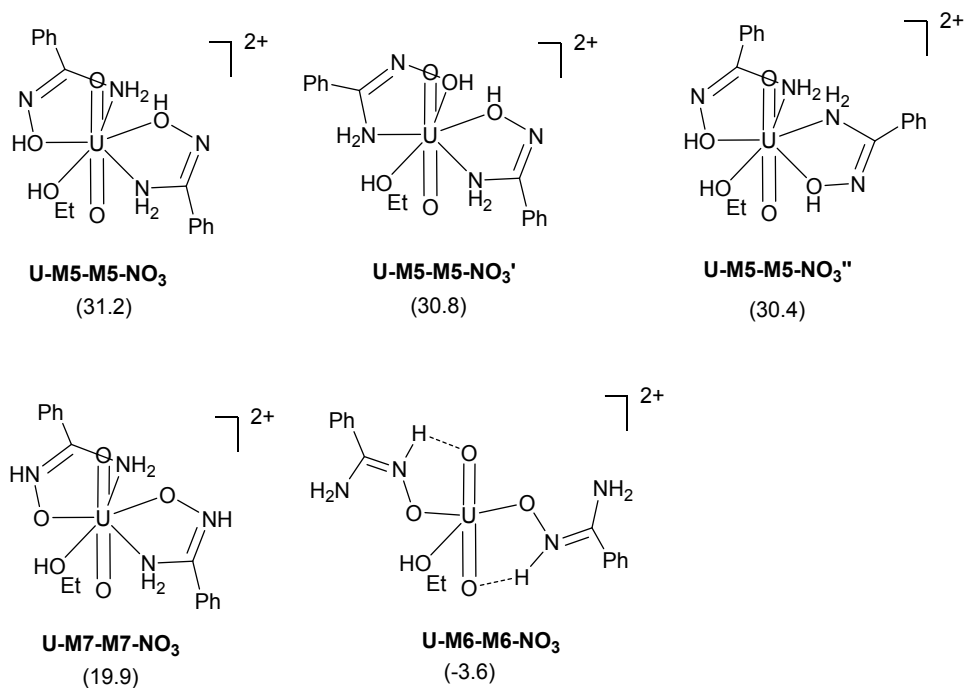


Figure S11. The possible complexes formed via the ligand exchange of **AO1/TAO1** with NO_3^- on **U-EtOH**.

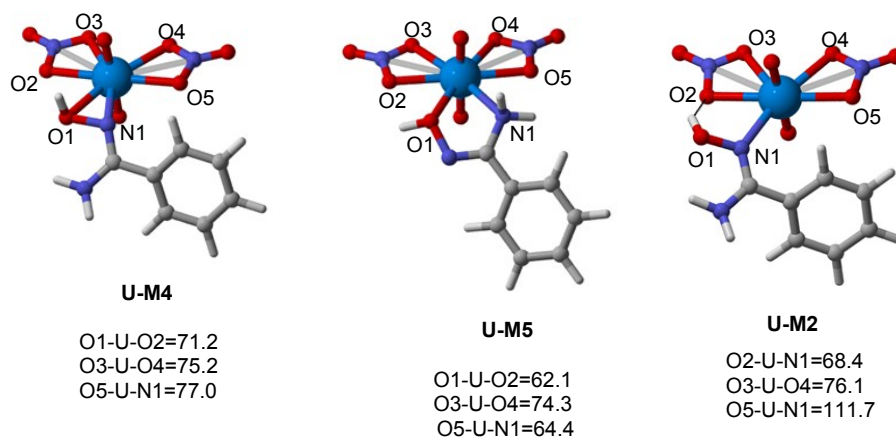


Figure S12. The comparison between the structure of **U-M5**, **U-M4**, and **U-M2**. *The large chelating angle of AO1 ligand in U-M5 results in the crowded equatorial plane of the uranium center.*

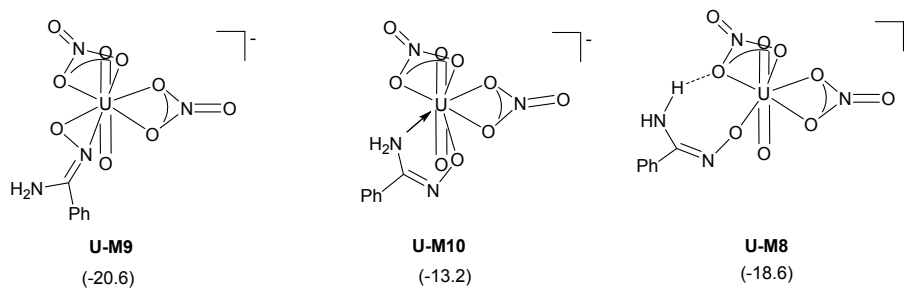


Figure S13. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1})$ complexes.

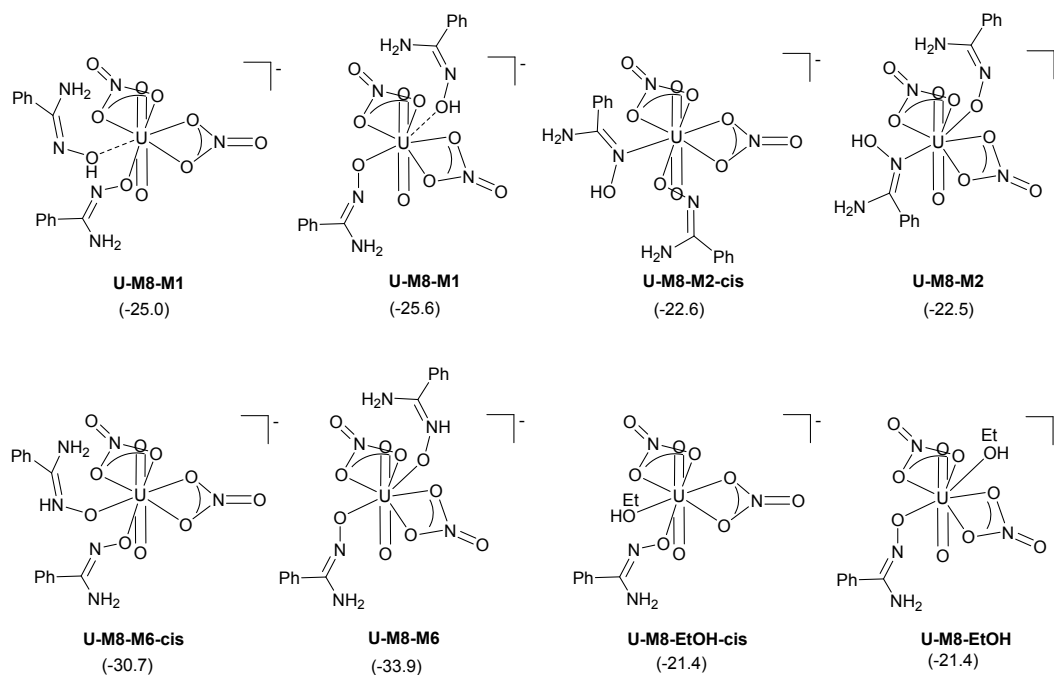


Figure S14. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1})(\text{Neu})$ complexes.

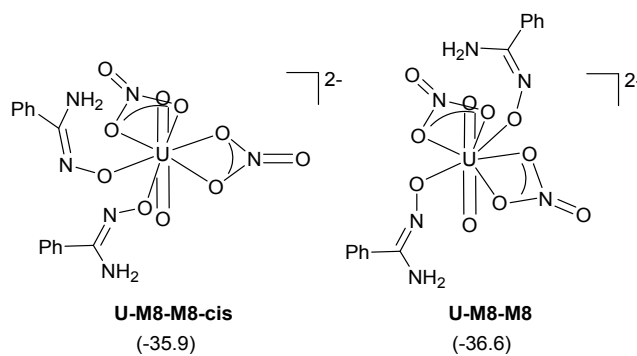


Figure S15. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1})_2$ complexes with double **M8** modes.

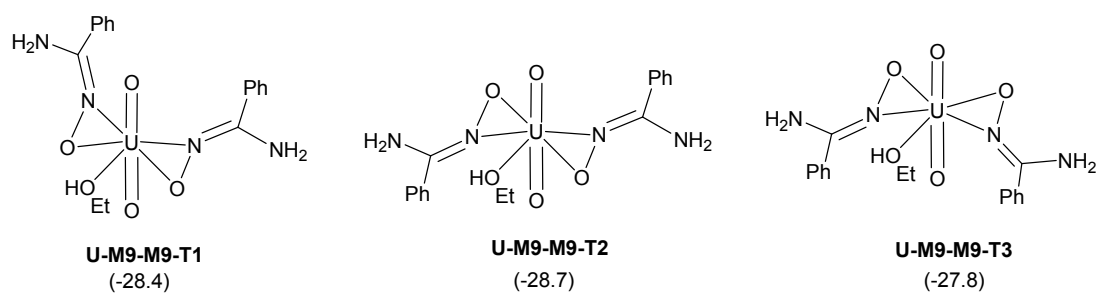


Figure S16. The comparisons between different $\text{UO}_2(\text{EtOH})(\text{AAO1})_2$ complexes with double **M9** modes.

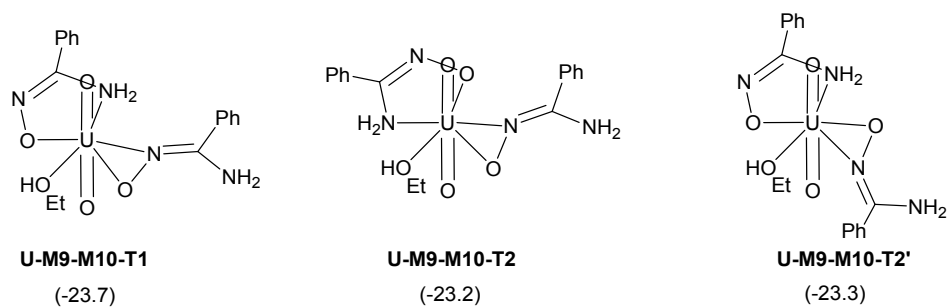


Figure S17. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1})_2$ complexes with one **M9** and one **M10** modes.

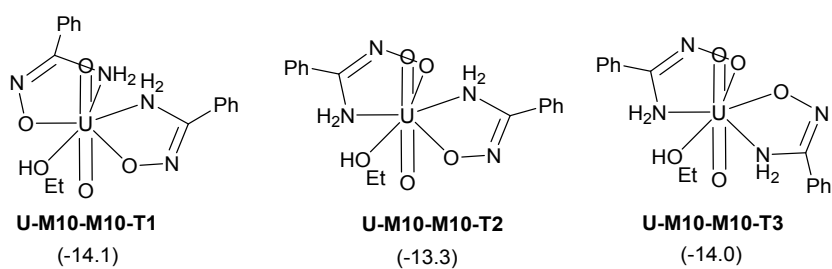


Figure S18. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1})_2$ complexes with double **M10** modes.

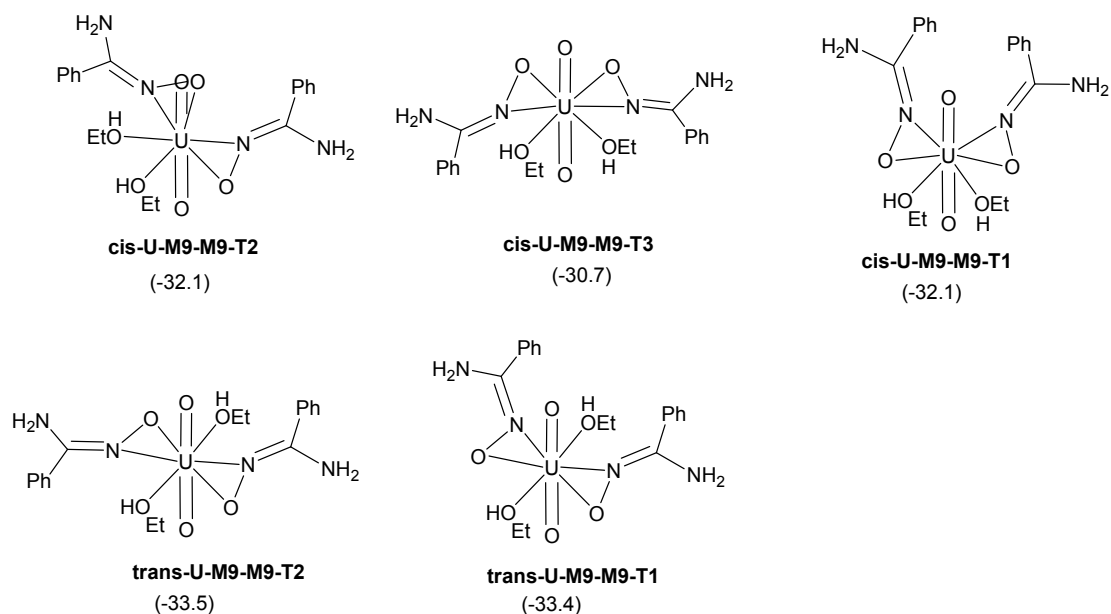


Figure S19. The comparison between different $\text{UO}_2(\text{EtOH})_2(\text{AAO1})_2$ complexes (AAO1 is ligated via **M9** mode).

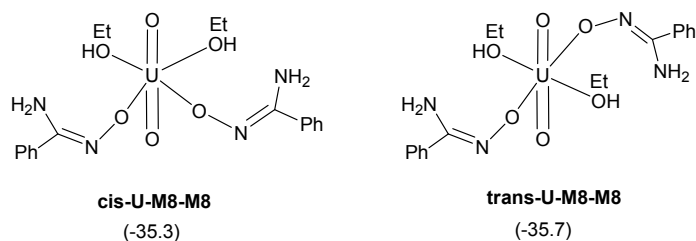


Figure S20. The comparison between different $\text{UO}_2(\text{EtOH})_2(\text{AL1})_2$ complexes with double mono-O coordinated AL1 ligands.

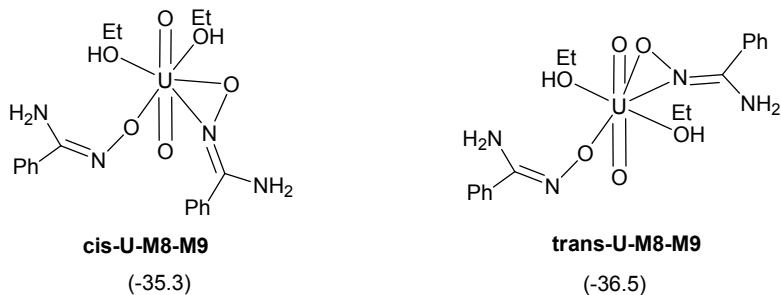


Figure S21. The comparison between different $\text{UO}_2(\text{EtOH})_2(\text{AAO1})_2$ complexes with one **M8** and one **M9** AAOs.

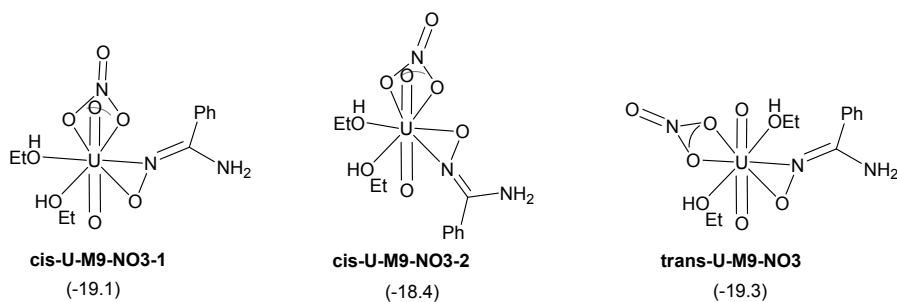


Figure S22. The comparison between different $\text{UO}_2(\text{EtOH})_2(\text{NO}_3)(\text{AAO1})$ complexes (via **M9**).

Table S2. The possible coordination modes of AAO1' and AAO1'', and the symbol for each of them in the nomenclature of the formed uranyl complexes.

Binding modes of AAO1'			
Symbol	M11	M12	M13
Binding modes of AAO1''			
Symbol	M14	M15	M16

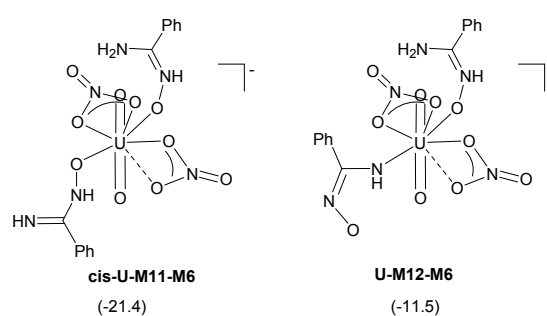


Figure S23. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')(\text{TAO1})$ complexes.

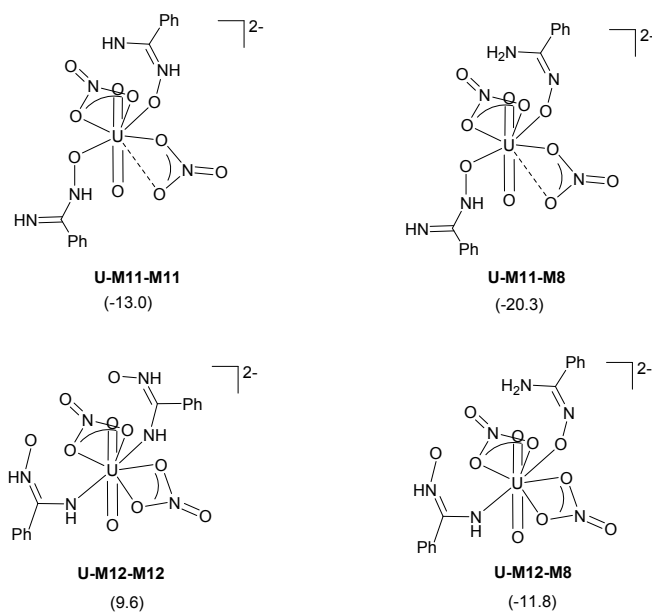


Figure S24. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')_2$ and $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')(\text{AAO1})$ complexes.

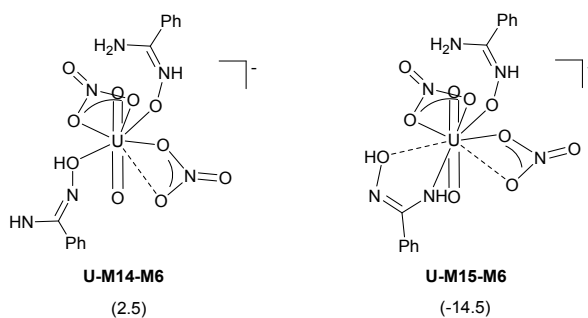


Figure S25. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')(\text{TAO1})$ complexes.

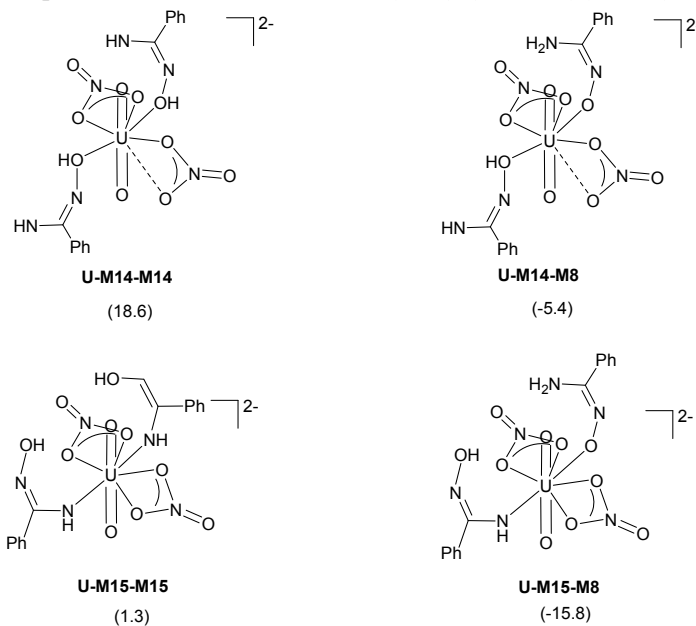


Figure S26. The comparison between different $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')_2$ and $\text{UO}_2(\text{NO}_3)_2(\text{AAO1}')(\text{AAO1})$ complexes.

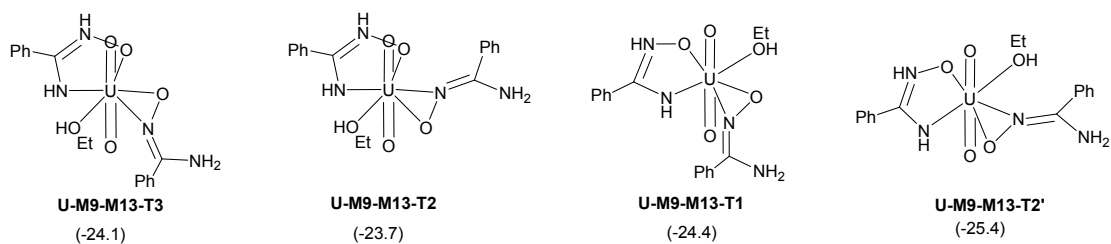


Figure S27. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1}')(\text{AAO1})$ complexes (AAO1' is coordinated with M13 mode, and AAO1 is coordinated with M9 mode).

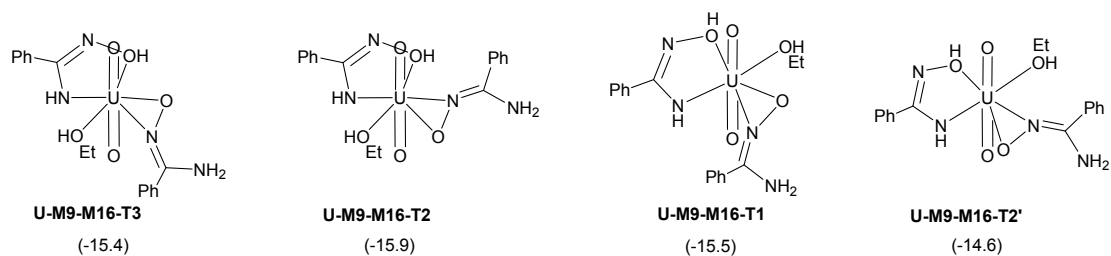


Figure S28. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1}'')(\text{AAO1})$ complexes ($\text{AAO1}''$ M16, and AAO1 is coordinated with M9 mode).

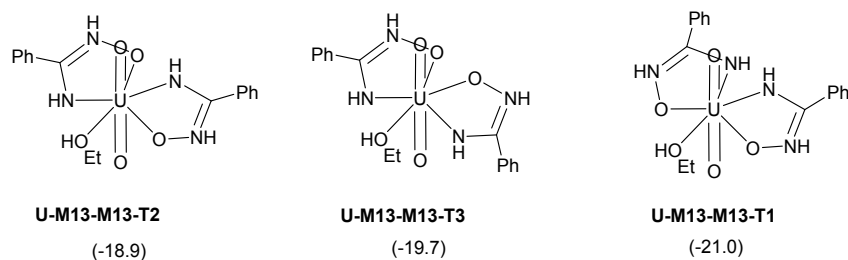


Figure S29. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1}')_2$ complexes (both $\text{AAO1}'$ are coordinated with chelated modes).

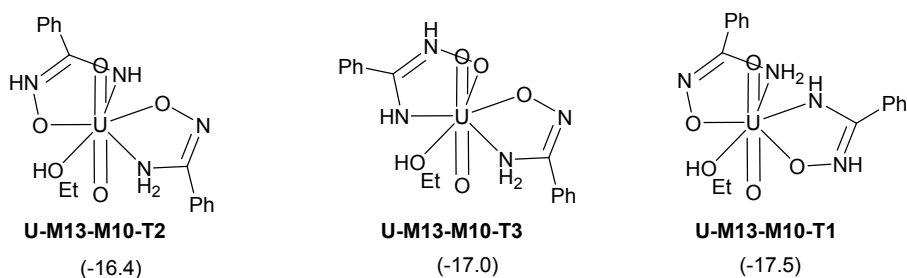


Figure S30. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1}')(\text{AAO1})$ complexes (both $\text{AAO1}'$ and AAO1 are coordinated with the chelated modes)

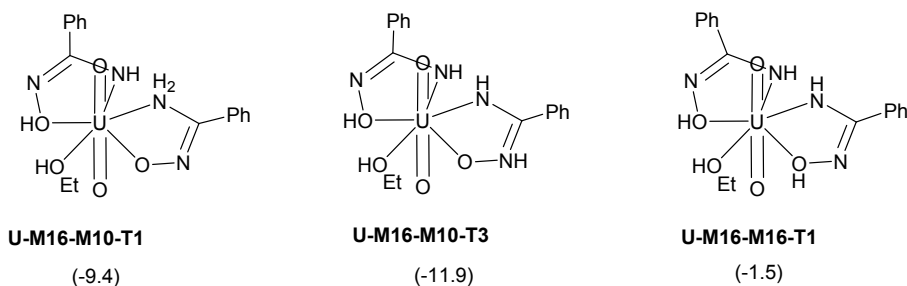


Figure S31. The comparison between different $\text{UO}_2(\text{EtOH})(\text{AAO1}'')(\text{AAO1})$ (both $\text{AAO1}''$ and AAO1 are coordinated with the chelated modes)

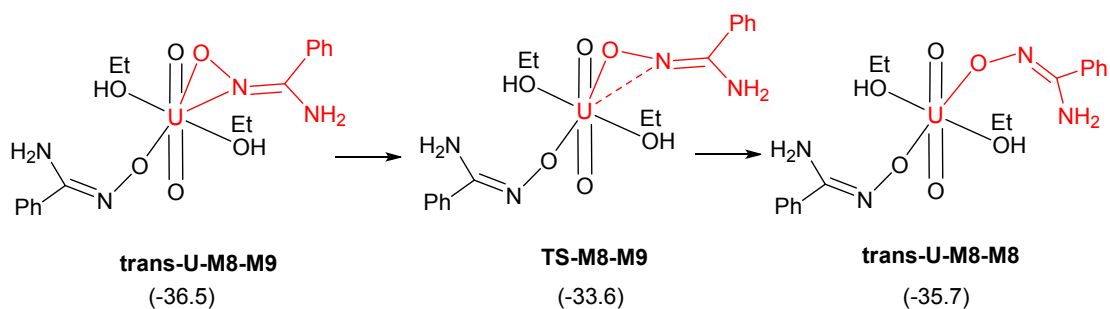


Figure S32. The kinetic transformation of **trans-U-M8-M9** to **trans-U-M8-M8** via the transition state of **TS-M8-M9**.

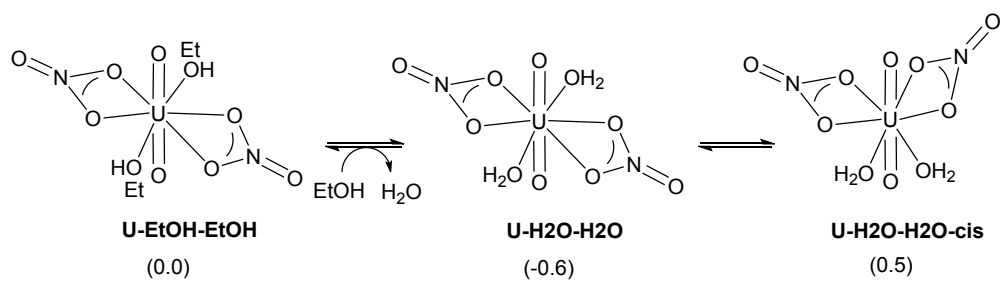


Figure S33. The ligand exchange reactions between H_2O and EtOH on $\text{UO}_2(\text{NO}_3)_2(\text{EtOH})_2$.

2. The relative enthalpies calculated for AAO1, AAO1', and AAO1''.

Due to the lack of the absolute energy of H⁺, the relative enthalpy of AAO1, AAO1' and AAO1'' are calculated via the following strategies.

First, similar to our recent studies on predicting the pKa of different organic molecules, the isodesmic reaction (1) has been first designed:



So that

$$\ln K_a = -\frac{\Delta G_{exchange}}{RT} \quad (2)$$

On the basis of eqs 1 and 2, we got

$$e^{-\Delta G_{exchange}/RT} = \frac{[\mathbf{EtO}^-][\mathbf{AO1}]}{[\mathbf{EtOH}][\mathbf{AAO1}]} \quad (3)$$

Using the experimental pKa data of EtOH in H₂O (i.e. 15.9), we have:

$$pKa(\mathbf{AO1}) = 15.9 + \frac{\Delta G_{exchange}}{2.303RT} \quad (4)$$

With eq.4 and the generated $\Delta G_{exchange}$, we got the pKa value of AO1. The Gibbs free energy change (ΔG^0) of the reaction $\mathbf{AO1} \rightarrow \mathbf{AAO1} + \mathbf{H}^+$ could then be generated from the pKa value and the equation (5).

$$pKa(\mathbf{AO1}) = -\frac{\Delta G^0}{2.303RT} \quad (5)$$

The entropic effect might be negligible in the concerned reaction system. For example, for equation 1, $\Delta G_{exchange} = -14.2$ kcal/mol, and $\Delta H_{exchange} = -14.6$ kcal/mol. Therefore, $\Delta G^0(\mathbf{AAO1})$ data is used as $\Delta H^0(\mathbf{AAO1})$ in our system.

3. Comparison between the calculation results with B3LYP and B3LYP-D3.

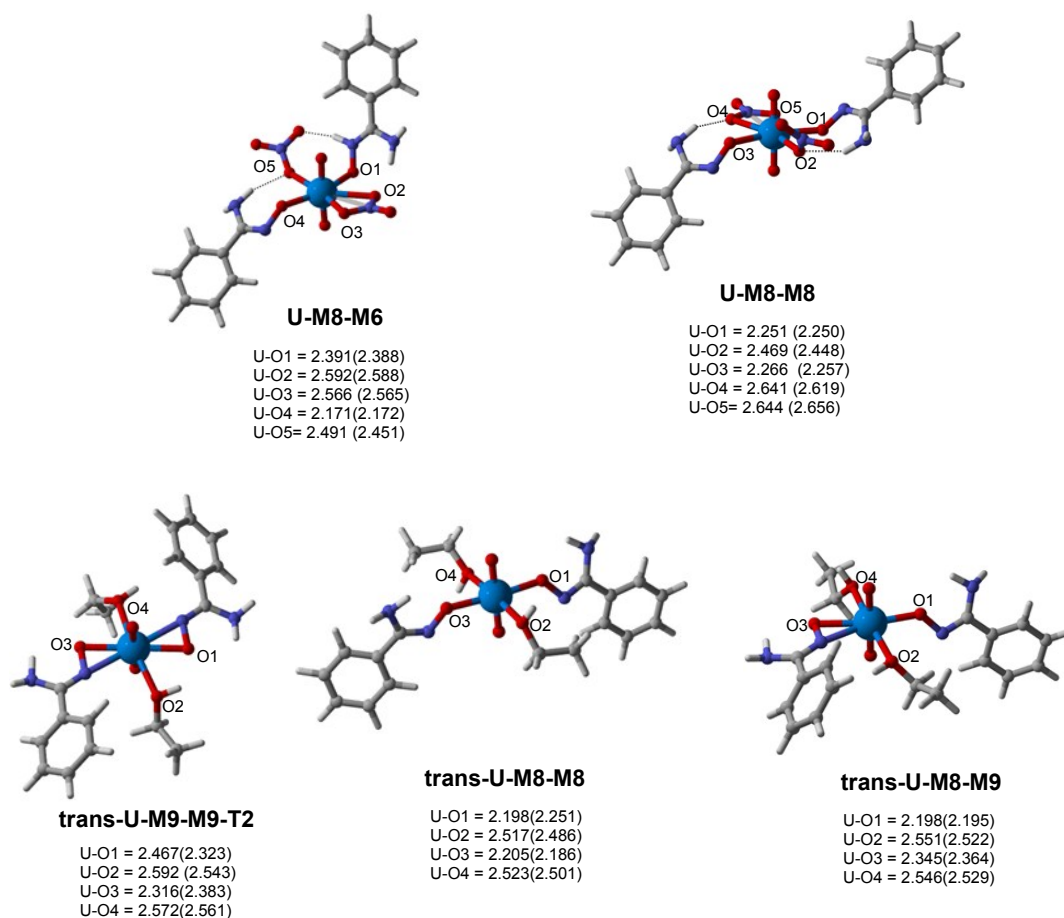


Figure S34. The optimized structure and the selected structural parameters of the most stable structures with B3LYP and B3LYP-D3 (in parenthesis) methods. The bond distances are given in angstrom.

Table 2. The relative enthalpies of the most stable structures (in kcal/mol).

	U-M8-M6	U-M8-M8		
$\Delta H(\text{B3LYP})$	-33.9	-36.6		
$\Delta H(\text{B3LYP-D3})$	-30.3	-33.1		
	Trans-U-M9-M9-T2	Trans-U-M8-M8	Trans-U-M8-M9	
$\Delta H(\text{B3LYP})$	-33.5	-35.7	-36.5	
$\Delta H(\text{B3LYP-D3})$	-36.3	-29.0	-30.2	

4. Thermal correction to enthalpy (TCE), and total electronic energy (E) in water solvent for all species (in hartree).

Complex	TCG	TCE	E	ΔH	ΔG	Complex	TCG	TCE	E	ΔH	ΔG
UO₂(NO₃)₂	-0.002659	0.050222	-1188.549988	20.3	-1.6	U-EtOH	0.070714	0.137805	-1343.670209	6.1	-5.5
U-EtOH-EtOH	0.146667	0.225937	-1498.778067	0.0	0.0	U-EtOH-EtOH-cis	0.146816	0.225813	-1498.776862	0.7	0.8
U-M2	0.128774	0.206083	-1644.949069	3.7	-5.7	U-M2'	0.127546	0.206041	-1644.946973	5.0	-5.2
U-M5	0.130037	0.206175	-1644.943271	7.4	-1.3	U-M4	0.127719	0.205711	-1644.951254	2.1	-7.8
U-M6	0.126853	0.206239	-1644.965779	-6.6	-17.4	U-M2-EtOH	0.202538	0.293861	-1800.056651	-2.4	-1.5
U-M2-EtOH-cis	0.204542	0.294073	-1800.056104	-1.9	0.1	U-M1-EtOH	0.201165	0.29359	-1800.056772	-2.1	-2.3
U-M1-EtOH-cis	0.202433	0.29343	-1800.054399	-0.7	0.0	U-M6-EtOH	0.203914	0.294253	-1800.074431	-13.3	-11.8
U-M6-EtOH-cis	0.203856	0.294226	-1800.070995	-11.2	-9.7	U-M2-M2	0.259232	0.361821	-2101.335757	-5.1	-2.8
U-M2-M2-cis	0.261669	0.362112	-2101.334092	-3.9	-0.2	U-M1-M1-cis	0.259184	0.361094	-2101.337008	-6.4	-3.6
U-M1-M1	0.257090	0.361105	-2101.336575	-6.1	-4.6	U-M1-M2	0.261000	0.360769	-2101.334868	-5.2	-1.1
U-M1-M2-cis	0.259939	0.361584	-2101.335353	-5.0	-2.1	U-M6-M6	0.258897	0.362126	-2101.364763	-23.1	-21.2
U-M6-M6-cis	0.259368	0.362088	-2101.364763	-23.1	-20.9	U-M2-M6	0.260827	0.362287	-2101.351556	-14.7	-11.7
U-M2-M6-cis	0.261408	0.362319	-2101.350743	-14.2	-10.8	U-M5-M5-NO3	0.312689	0.407588	-1695.311489	31.2	20.4
U-M5-M5-NO3'	0.313572	0.407637	-1695.312222	30.8	20.5	U-M5-M5-NO3''	0.313105	0.407679	-1695.312885	30.4	19.8
U-M7-M7-NO3	0.315513	0.409429	-1695.331325	19.9	9.7	U-M6-M6-NO3	0.310546	0.409077	-1695.368577	-3.6	-16.7
U-M4	0.127719	0.205711	-1644.951254	2.1	-7.8	U-M9	0.116874	0.192831	-1644.505297	-20.6	-29.9
U-M10	0.116395	0.192503	-1644.49308	-13.2	-22.5	U-M8	0.114261	0.192528	-1644.501773	-18.6	-29.3
U-M8-M1-cis	0.244418	0.348191	-2100.884475	-25.0	-24.0	U-M8-M1	0.241011	0.348137	-2100.885326	-25.6	-26.7
U-M8-M2-cis	0.245062	0.348004	-2100.880507	-22.6	-21.1	U-M8-M2	0.245283	0.348195	-2100.880549	-22.5	-21.0
U-M8-M6-cis	0.247081	0.34786	-2100.893152	-30.7	-27.8	U-M8-M6	0.246137	0.348363	-2100.898893	-33.9	-32.0
U-M8-M8-cis	0.228616	0.333678	-2100.418031	-35.9	-36.3	U-M8-M8	0.224928	0.333792	-2100.419249	-36.6	-39.4

U-M9-M9-T2	0.287933	0.382109	-1694.44269	-28.7	-40.1	U-M9-M9-T3	0.288968	0.38219	-1694.441442	-27.8	-38.7
U-M9-M9-T1	0.289190	0.382251	-1694.442448	-28.4	-39.2	U-M9-M10-T1	0.288716	0.382014	-1694.434607	-23.7	-34.6
U-M9-M10-T2	0.288993	0.381959	-1694.433887	-23.2	-34.0	U-M9-M10-T3	0.287270	0.381997	-1694.43404	-23.3	-35.1
U-M10-M10-T1	0.288374	0.381798	-1694.419174	-14.1	-26.8	U-M10-M10-T3	0.285014	0.38133	-1694.418486	-14.0	-26.8
U-M10-M10-T2	0.287612	0.381942	-1694.417959	-13.3	-24.8	Cis-U-M9-M9-T2	0.364534	0.469912	-1849.54601	-32.1	-31.4
Cis-U-M9-M9-T3	0.365938	0.469707	-1849.543578	-30.7	-29.0	Cis-U-M9-M9-T1	0.365041	0.46989	-1849.545898	-32.1	-31.0
Trans-U-M9-M9-T2	0.365050	0.469943	-1849.548245	-33.5	-32.5	Trans-U-M9-M9-T1	0.365654	0.469764	-1849.547812	-33.4	-31.8
Cis-U-M8-M8	0.361252	0.469059	-1849.550253	-35.3	-36.1	Trans-U-M8-M8	0.359098	0.469207	-1849.550993	-35.7	-38.0
Cis-U-M8-M9	0.361535	0.469479	-1849.550544	-35.3	-36.1	Trans-U-M8-M9	0.360995	0.469433	-1849.552422	-36.5	-37.7
Cis-U-M9-NO3-1	0.254961	0.347874	-1674.166786	-19.1	-19.1	Cis-U-M9-NO3-2	0.255370	0.347606	-1674.165439	-18.4	-18.0
Trans-U-M9-NO3	0.255802	0.347885	-1674.16714	-19.3	-18.8	U-M11-M6	0.246393	0.348432	-2100.878912	-21.4	-19.3
U-M12-M6	0.248110	0.348553	-2100.863338	-11.5	-8.4	U-M11-M11	0.230320	0.334247	-2100.382071	-13.0	-12.7
U-M11-M8	0.230112	0.33394	-2100.393424	-20.3	-19.9	U-M12-M12	0.230599	0.33363	-2100.345402	9.6	10.5
U-M12-M8	0.230875	0.333775	-2100.3797	-11.8	-10.8	U-M14-M6	0.243413	0.346612	-2100.839105	2.5	3.9
U-M15-M6	0.248854	0.348568	-2100.868167	-14.5	-11.0	U-M14-M14	0.227178	0.332427	-2100.32981	18.6	18.1
U-M14-M8	0.228882	0.332975	-2100.3686	-5.4	-5.1	U-M15-M15	0.230268	0.333104	-2100.358129	1.3	2.3
U-M15-M8	0.231386	0.333513	-2100.385704	-15.8	-14.3	U-M9-M13-T3	0.288822	0.382142	-1694.43539	-24.1	-35.0
U-M9-M13-T2	0.288685	0.382314	-1694.435019	-23.7	-34.9	U-M9-M13-T1	0.290490	0.382521	-1694.436234	-24.4	-34.5
U-M9-M13-T2'	0.288484	0.382178	-1694.437592	-25.4	-36.6	U-M9-M16-T3	0.287900	0.381439	-1694.420891	-15.4	-26.5
U-M9-M16-T2	0.285966	0.381411	-1694.421677	-15.9	-28.2	U-M9-M16-T1	0.286904	0.381442	-1694.420955	-15.5	-27.1
U-M9-M16-T2'	0.286556	0.381328	-1694.419499	-14.6	-26.5	U-M13-M13-T2	0.290137	0.382419	-1694.427358	-18.9	-29.1
U-M13-M13-T3	0.289395	0.382089	-1694.428286	-19.7	-30.2	U-M13-M13-T1	0.289272	0.38218	-1694.430559	-21.0	-31.7
U-M13-M10-T2	0.288898	0.382161	-1694.423209	-16.4	-208.6	U-M13-M10-T3	0.287706	0.381804	-1694.423807	-17.0	-209.0

U-M13-M10-T1	0.290199	0.382187	-1694.424869	-17.5	-27.5	U-M16-M10-T1	0.288126	0.381238	-1694.411089	-9.4	-20.2
U-M16-M10-T3	0.288086	0.381538	-1694.415353	-11.9	-20.2	U-M16-M16-T1	0.286950	0.380466	-1694.3978	-1.5	-20.2
U-EtOH-EtOH	0.146667	0.225937	-1498.778067	0.0	0.0	U-H2O-H2O	0.041995	0.106023	-1341.509397	-0.6	2.1
U-H2O-H2O-cis	0.042791	0.106429	-1341.508057	0.5	3.4	TS-M8-M9	0.362425	0.468266	-1849.546711	-33.6	-33.2

5. Cartesian coordinates for the examined structures.

UO₂(NO₃)₂

U	0.0000200	0.00002300	-0.00003900
O	-0.00027000	1.75223000	0.00003500
O	0.00024800	-1.75217700	-0.00031800
O	2.16642400	-0.00005400	1.08094100
O	2.16689900	0.00024300	-1.08094900
O	4.06674600	-0.00013900	0.00034000
N	2.87688700	0.00001100	0.00004600
O	-2.16648200	-0.00023600	1.08095300
N	-2.87688600	-0.00009600	0.00007000
O	-2.16684500	0.00004000	-1.08093600
O	-4.06674600	-0.00009100	0.00028300

U-ETOH

U	0.0000200	0.00002300	-0.00003900
O	-0.00027000	1.75223000	0.00003500
O	0.00024800	-1.75217700	-0.00031800
O	2.16642400	-0.00005400	1.08094100
O	2.16689900	0.00024300	-1.08094900
O	4.06674600	-0.00013900	0.00034000
N	2.87688700	0.00001100	0.00004600
O	-2.16648200	-0.00023600	1.08095300
N	-2.87688600	-0.00009600	0.00007000
O	-2.16684500	0.00004000	-1.08093600
O	-4.06674600	-0.00009100	0.00028300

U-EtOH-EtOH

U	0.00001200	0.06622600	0.00012000
O	-0.16728300	0.07347500	1.75369800
O	-1.06878400	-2.17261800	-0.11222000
O	2.52664500	0.19434200	0.17942400
O	1.06974300	-2.17213500	0.11211800
N	0.00063400	-2.87654300	-0.00008200
O	0.00092100	-4.07439200	-0.00022400
O	0.16728900	0.07416900	-1.75345800
O	1.06735800	2.34417100	0.10202100
O	-2.52671600	0.19332100	-0.17917500
O	-1.06822600	2.34373800	-0.10168500

N	-0.00055400	3.04928300	-0.00002000
O	-0.00076100	4.24682600	-0.00028300
H	2.77516000	1.12501200	0.25928400
H	-2.77566800	1.12391000	-0.25862300
C	-3.57988600	-0.54195000	0.50066500
C	-4.88551200	-0.45282000	-0.26749300
H	-3.67823400	-0.15041600	1.51774300
H	-3.21703100	-1.56545300	0.55444500
H	-5.65525000	-1.03977500	0.24100000
H	-5.24401700	0.57915500	-0.33286100
H	-4.76498200	-0.84433500	-1.27951400
C	3.57976200	-0.54000100	-0.50150300
C	4.88534100	-0.45231600	0.26691500
H	3.67825500	-0.14685700	-1.51794500
H	3.21675400	-1.56336200	-0.55694800
H	5.65503000	-1.03857700	-0.24245400
H	5.24398700	0.57949600	0.33399500
H	4.76463400	-0.84544700	1.27828600

U-EtOH-EtOH-cis

U	0.03188200	-0.25537400	-0.00790300
O	0.26773900	-0.21435300	1.73968300
O	2.45536900	-0.02304700	-0.39272100
O	1.71000600	-2.03879800	-0.27463200
O	3.83935400	-1.69886600	-0.62883300
N	2.73176400	-1.28543000	-0.44316400
O	-0.26538500	-0.21101700	-1.74485900
O	-2.34092400	-0.87186200	0.40427600
O	-0.97526100	-2.51674000	0.16509400
O	-3.08292600	-2.92229900	0.57153700
O	0.79714600	2.19666000	-0.04269700
N	-2.17958000	-2.15799200	0.39098900
H	0.16220000	2.67941300	0.50143000
O	-1.75729000	1.66171900	0.28765700
H	-2.40680900	1.23837800	0.86738900
C	-2.46587200	2.16417500	-0.88628700
C	-3.48469200	3.22068000	-0.50327100
H	-2.93032400	1.31840400	-1.39800300
H	-1.68444500	2.56840600	-1.52878900
H	-3.97253000	3.60630000	-1.40245500
H	-4.26358500	2.80544500	0.14293600
H	-3.01164300	4.05700200	0.01651400
C	2.08122600	2.87876700	-0.05087000
C	2.69151300	2.95712900	1.33596000

H	1.92624200	3.87084000	-0.48545700
H	2.70436000	2.29547400	-0.72375200
H	3.65730300	3.46767600	1.28625600
H	2.05302700	3.51821500	2.02566500
H	2.85208700	1.95711900	1.74135200

U-M2

U	0.74683500	0.17606500	-0.05518300
O	0.10968600	0.25964100	1.58251400
O	-0.17349900	-2.93988100	-1.17349200
O	1.32714400	0.06540800	-1.71229400
O	1.73394700	2.43330100	0.16590800
O	-0.28199400	2.32755000	-0.59920000
O	0.68487700	4.27381400	-0.36772400
N	0.71928600	3.08195600	-0.27020600
O	3.04104500	-0.25605400	0.74093000
N	2.98781400	-1.53341800	0.75648900
H	0.71077500	-2.94669600	-0.77041200
N	-0.78620600	-1.78115400	-0.64361600
C	-2.06802300	-1.96436200	-0.48235200
N	-2.66098700	-3.16010800	-0.66839300
H	-3.65972500	-3.21408000	-0.76799100
H	-2.08634700	-3.92406100	-0.99059100
C	-2.88749500	-0.80886600	-0.05950300
C	-3.80739800	-0.94001700	0.98939900
C	-2.73353200	0.42797600	-0.69622900
C	-4.54811200	0.16130700	1.40118800
H	-3.91329000	-1.89078100	1.49875800
C	-3.47046800	1.53094000	-0.27084400
H	-2.07176000	0.52029500	-1.55075500
C	-4.37791500	1.39729000	0.77545700
H	-3.32650600	2.48715400	-0.75751100
O	1.81999300	-2.00409400	0.43884800
O	3.91068700	-2.23745600	1.03980300
H	-5.24744300	0.06102100	2.22288800
H	-4.95134200	2.25476700	1.10747400

U-M2'

U	-0.93221700	0.09990900	-0.01082000
O	0.04200600	0.25939000	-1.46573400
O	0.41734500	-1.43848400	2.62756900
O	-1.84772000	-0.09319400	1.49589500
O	-1.91945900	2.31250200	-0.37471100

O	-0.09889100	2.28930100	0.78512600
O	-1.08179900	4.19387500	0.35570300
N	-1.03715900	3.00266900	0.26091600
O	-2.68796700	-1.04825900	-1.25699400
N	-2.23535600	-2.24939700	-1.12196400
H	-0.49012200	-1.11328500	2.71128400
N	0.90602100	-0.78022900	1.46748300
C	2.17671100	-1.05649800	1.30500600
N	2.81782900	-1.92561700	2.10647900
H	2.30932800	-2.34784000	2.86807400
H	3.82153100	-1.97722900	2.08685700
C	2.94313800	-0.41370200	0.21404600
C	3.74970600	-1.19804400	-0.62149400
C	2.89469900	0.97309400	0.03456000
C	4.48947000	-0.59866900	-1.63445500
H	3.76977900	-2.27480000	-0.49743500
C	3.64254500	1.56515100	-0.97870600
H	2.28351200	1.58529600	0.68561400
C	4.43762300	0.78326100	-1.81289700
H	3.60173200	2.63928700	-1.11415900
O	-1.14686400	-2.31860900	-0.43694300
O	-2.77755700	-3.20664300	-1.58963200
H	5.09800000	-1.21012000	-2.29022700
H	5.01478700	1.24846800	-2.60359200

U-M5

U	1.06981400	0.06103600	0.08310600
O	0.45274900	-0.16157600	-1.55241300
O	1.56053300	0.26264300	1.76557800
O	3.33415400	-0.64670100	-0.59124900
O	2.00605100	-2.21745700	0.05023600
O	4.03736600	-2.71572000	-0.58591100
N	3.18247500	-1.90330000	-0.38975900
O	2.24436500	2.12092300	-0.57031100
N	1.28910000	2.94490300	-0.34198500
O	0.21112600	2.37864200	0.09654200
O	1.37601800	4.12519800	-0.51422000
N	-1.84961800	-1.89528400	0.49017100
O	-0.47417100	-1.91111100	0.84747000
C	-2.29841700	-0.69659800	0.55510800
N	-1.44144000	0.36220900	0.98293800
C	-3.68589800	-0.42042300	0.13821300
C	-4.32103200	-1.26707700	-0.78270900

C	-4.38675900	0.67523400	0.65972600
C	-5.63181800	-1.01978300	-1.16703100
H	-3.77301700	-2.10425700	-1.19478900
C	-5.70002900	0.91826300	0.26945000
H	-3.92355500	1.33034100	1.38887900
C	-6.32414100	0.07286000	-0.64401200
H	-6.11267800	-1.67402500	-1.88458300
H	-6.23441900	1.76582900	0.68165400
H	-7.34514000	0.26634900	-0.95160900
H	-1.80059400	1.28662500	0.76693200
H	-1.22808200	0.30491900	1.97780000
H	-0.16595500	-2.80434600	0.64212000

U-M4

U	0.98929400	0.08091400	0.06359700
O	1.35242600	0.28222200	1.78142800
O	-0.79970400	1.76968300	0.24481200
O	1.14770500	2.49666000	-0.33637200
O	-0.51411600	3.90185300	-0.13940000
N	-0.07732900	2.78790200	-0.08146300
O	0.56240800	-0.22820100	-1.61995000
O	2.79892400	-1.57052200	-0.08358600
O	3.34699900	0.46830400	-0.53371600
O	4.86575300	-1.10022800	-0.61693700
N	3.73722400	-0.74994700	-0.42345500
O	0.05585100	-2.27557300	0.83044000
N	-1.01140200	-1.28777000	0.77152000
C	-2.09374500	-1.80378200	0.23545600
N	-2.18127800	-3.08684600	-0.13813400
C	-3.25522500	-0.90824700	0.05026400
H	-3.06666600	-3.48433600	-0.39939300
H	-1.36792500	-3.67789400	-0.06217800
C	-4.14025900	-1.11279600	-1.01774500
C	-3.46476500	0.15860000	0.93209500
C	-5.22913800	-0.26651700	-1.18994300
C	-4.55543000	1.00059600	0.75257800
H	-2.77217300	0.32492100	1.74561600
C	-5.43966900	0.78815400	-0.30297300
H	-4.70932700	1.82822300	1.43402700
H	-6.28686400	1.44972600	-0.44147200
H	0.31728500	-2.29591700	1.76393700
H	-3.95731200	-1.90137900	-1.73879200
H	-5.90313000	-0.42043000	-2.02411200

U-M6

U	-1.39032400	-0.00056100	0.10987900
O	-0.40049500	0.01656700	-1.37113200
O	0.66849000	-0.29536700	1.12948500
O	-2.26711000	-0.03328000	1.63931500
O	-1.53439800	-2.45583300	-0.03973500
O	-3.12422900	-1.35665500	-1.00615600
O	-3.12988300	-3.54060700	-1.06508600
N	-2.62635600	-2.50861500	-0.72374100
O	-0.82484000	2.38476500	0.44165100
N	-1.84091300	2.87028100	-0.18527800
N	1.80049200	-0.22804100	0.40736800
C	2.96861300	-0.28230300	0.99690500
N	3.00097500	-0.48881600	2.32036900
H	2.10996900	-0.53167900	2.79861800
H	3.83613700	-0.27936800	2.83993100
C	4.20137100	-0.14715300	0.20240800
C	4.27049400	0.78598100	-0.84112300
C	5.31113500	-0.95272400	0.49178400
C	5.43638700	0.90193500	-1.59013900
H	3.43000400	1.43919900	-1.04534000
C	6.47322300	-0.82790600	-0.26090100
H	5.25220500	-1.69340100	1.28082500
C	6.53700800	0.09728900	-1.30179500
H	7.32550600	-1.45969700	-0.04142600
O	-2.63896900	1.98019400	-0.66021300
O	-2.02342300	4.04775200	-0.31462300
H	5.48789300	1.62893200	-2.39156000
H	7.44425400	0.19189100	-1.88673000
H	1.69394900	-0.18896300	-0.60506600

U-M2-EtOH

U	0.66826700	0.04445800	0.17104100
O	-0.04396800	0.20882300	-1.42960600
O	-1.27490500	-0.50468900	2.87287000
O	1.34345400	-0.11082700	1.80874500
O	1.76963300	-2.06073500	-0.53612700
O	-0.19850700	-2.30200300	0.29242700
O	0.89911600	-4.06038500	-0.40030000
N	0.82337300	-2.87663300	-0.22333400
O	1.65596600	2.33925400	-0.06106600
N	0.65906000	3.01977900	0.38804200
H	-0.32122600	-0.38333400	2.97579400

N	-1.50529800	-0.19090600	1.50835400
C	-2.75338300	-0.41148000	1.20832300
N	-3.61682300	-0.95957400	2.09190900
H	-4.60481100	-0.90189100	1.91770000
H	-3.28791700	-1.14929600	3.02546900
O	-0.32054600	2.29309600	0.77369500
O	0.65841100	4.21808900	0.43739200
C	-3.26852400	-0.08195900	-0.14211200
C	-3.09721200	1.19840100	-0.67807100
C	-3.97182300	-1.05325100	-0.86627700
C	-3.62381200	1.49873600	-1.93107700
C	-4.48848000	-0.74688100	-2.12044900
H	-4.08601700	-2.05036500	-0.45704400
C	-4.31712400	0.53021100	-2.65291900
H	-5.01712300	-1.50615100	-2.68499200
H	-4.72093300	0.76788600	-3.63047400
C	4.27933800	-0.42328700	-0.60569400
C	5.17732000	-0.21093400	-1.81142400
H	4.77167000	-0.11982200	0.32378900
H	3.97383200	-1.46239500	-0.51516700
H	6.09008600	-0.80373400	-1.70450100
H	4.66993300	-0.52021600	-2.72735300
H	5.47178300	0.83815400	-1.91371900
O	3.04332200	0.32245600	-0.74073900
H	3.23136300	1.26945200	-0.78246800
H	-2.55734300	1.94888200	-0.11464800
H	-3.48963900	2.49200900	-2.34311500

U-M2-EtOH-cis

U	-0.89487700	-0.12469400	0.05893900
O	-0.17183800	-0.52753600	-1.49527100
O	1.05545900	0.71455300	2.72762200
O	-1.54056700	0.34475300	1.64858900
O	-3.17704000	-0.33177300	-0.93010400
O	-2.29041100	1.61947000	-1.05792300
O	-4.26481600	1.27521100	-1.93351000
N	-3.30561600	0.86788300	-1.34300200
O	-1.94090500	-2.35883000	0.22023700
N	-0.97400400	-2.97067100	0.79370700
H	0.10667100	0.55401100	2.83672300
N	1.31769100	0.24900300	1.40773900
C	2.59845600	0.26868600	1.18091500
N	3.48203600	0.76618000	2.08475100
H	4.44765100	0.49604600	1.99776000

H	3.13039300	0.96887100	3.00852500
O	0.03984000	-2.20992200	1.04411100
O	-0.99812200	-4.13535500	1.07424000
C	3.14361900	-0.21470600	-0.11051100
C	2.79495900	-1.47461100	-0.60716700
C	4.05601600	0.58333200	-0.81432500
C	3.34822000	-1.92335400	-1.80315000
C	4.59985900	0.12961800	-2.01097700
H	4.31993500	1.56329200	-0.43333900
C	4.24648500	-1.12486900	-2.50643800
H	5.29386500	0.75626000	-2.55907100
H	4.67112500	-1.47775200	-3.43926900
C	0.14060700	3.31405200	0.70259600
C	0.87972500	4.52354700	0.15872400
H	-0.87255900	3.57457100	1.02364300
H	0.66520100	2.87116400	1.54705200
H	0.96308200	5.28904800	0.93527000
H	1.88544700	4.24949500	-0.16677600
H	0.34993400	4.96747300	-0.68929600
O	0.06045600	2.25889900	-0.29228200
H	-0.47406400	2.58358800	-1.03092800
H	2.10306600	-2.09705700	-0.05439500
H	3.07403900	-2.89982800	-2.18429800

U-M1-EtOH

U	-1.10748900	0.07235600	-0.29035800
O	-1.93025700	0.30922000	-1.82948100
O	-0.08630000	2.35678200	-0.57893500
O	-1.91735000	2.31701300	0.53540700
O	-0.87863600	4.21747700	0.24925700
N	-0.95680500	3.03380700	0.07875900
O	-0.22057300	-0.14176800	1.21571300
O	-0.40508800	-2.15120400	-1.17119700
O	-2.21349200	-2.12314500	-0.01022700
O	-1.52620900	-4.00444400	-0.88381700
O	1.09472000	0.06595300	-1.59370700
N	-1.38690600	-2.82912100	-0.70225600
H	0.93825900	-0.51929000	-2.34660900
O	-3.30797400	0.21706300	0.96368100
H	-3.46106500	1.13200500	1.23237700
N	2.32917100	-0.51506800	-1.04151200
C	3.05208500	0.41705000	-0.50416100
N	2.80655900	1.75281400	-0.52242300
C	4.30473400	-0.05142600	0.14816600

H	1.90729700	2.08280400	-0.84651900
H	3.24657700	2.31215300	0.18992500
C	5.45713100	0.74343700	0.11768600
C	4.34267300	-1.29492800	0.78954200
C	6.62821000	0.30266300	0.72730600
C	5.51595800	-1.73053600	1.39564100
H	3.44818500	-1.90347600	0.80885300
C	6.65952700	-0.93352100	1.36872000
H	5.53616300	-2.69244100	1.89485000
H	7.57172800	-1.27541400	1.84436100
H	5.44522900	1.69271200	-0.40531200
H	7.51758300	0.92134300	0.69310600
C	-4.34167200	-0.64880500	1.50046800
C	-4.32776900	-0.65207500	3.01866900
H	-4.12618700	-1.63332000	1.09419500
H	-5.30388400	-0.31087400	1.10431100
H	-5.10528700	-1.32260500	3.39531700
H	-3.36313600	-0.99752000	3.39592000
H	-4.52262400	0.34542600	3.42434600

U-M1-EtOH-cis

U	-1.29396900	-0.10178100	0.07640900
O	-2.03580600	0.06550900	1.66936100
O	-0.47768300	-2.38163500	0.67687500
O	-2.38335500	-2.31013400	-0.31027500
O	-1.50120900	-4.24947200	0.17430900
N	-1.46687100	-3.05184900	0.17411800
O	-0.45114800	-0.24963200	-1.46276800
O	-2.54968300	1.87874000	-0.75914200
O	-3.50780200	-0.01748600	-1.05765600
O	-4.49913000	1.80409400	-1.74616300
O	0.87905700	-0.21357300	1.40654700
N	-3.57955600	1.24590300	-1.22146000
H	0.78813300	0.02972200	2.33508300
O	-0.30783700	2.27242600	0.36363200
H	-0.99723700	2.83828700	-0.01192400
N	2.21706300	0.26956200	1.03814800
C	2.84787500	-0.67351100	0.40085900
N	2.42469800	-1.94303300	0.21519900
C	4.18717000	-0.29918000	-0.12700400
H	1.49641800	-2.22248600	0.51238800
H	2.85880500	-2.48887200	-0.51013200
C	5.24495700	-1.21540500	-0.07865300
C	4.40060400	0.97248100	-0.66987100

C	6.49830500	-0.86228100	-0.56959000
C	5.65500900	1.31961400	-1.16022100
H	3.57561200	1.67129900	-0.71329300
C	6.70512200	0.40428300	-1.11218900
H	5.81155700	2.30349300	-1.58712500
H	7.68128200	0.67673600	-1.49674100
H	5.09325100	-2.19258700	0.36512000
H	7.31424300	-1.57405600	-0.52202200
C	0.36667000	2.98131400	1.43238800
C	0.69257100	4.40571100	1.01915500
H	1.27601300	2.41401000	1.62172000
H	-0.26790300	2.96563200	2.32532400
H	1.22884300	4.91408700	1.82479600
H	1.32158800	4.41551600	0.12638900
H	-0.21573500	4.98011900	0.81178500

U-M6-EtOH

U	-1.02964300	0.04002100	-0.27579300
O	-0.09414700	0.06717300	1.22811500
O	0.93199600	-0.34247400	-1.46609700
O	-1.96531900	0.01249700	-1.77312600
O	0.24144600	2.19309900	-0.84879900
O	-1.63778500	2.46057800	0.15348400
O	-0.39481000	4.20389600	-0.27921300
N	-0.58254600	3.01717700	-0.32410600
O	-0.45271500	-2.42511500	-0.45579700
N	-1.45263700	-2.88289400	0.21007700
N	2.11421500	0.05805300	-0.98379400
C	2.93166900	-0.78409600	-0.40096200
N	2.58721100	-2.07733100	-0.33275200
H	1.64528800	-2.33914700	-0.61671300
H	3.05868300	-2.66458100	0.33473900
C	4.21770000	-0.29861900	0.13358100
C	4.28340900	0.92790500	0.80823300
C	5.37879900	-1.06603300	-0.02751000
C	5.50109700	1.38316000	1.30290600
H	3.38138800	1.50588000	0.97353100
C	6.59125000	-0.60502900	0.47337000
H	5.33454700	-2.00533800	-0.56642400
C	6.65470500	0.61949600	1.13659400
H	7.48812200	-1.19791600	0.33854800
O	-2.27597800	-1.97983200	0.58970900
O	-1.59699200	-4.05151200	0.45335800

H	5.54486800	2.32874500	1.82989400
H	7.60111300	0.97601000	1.52603100
H	2.34741200	1.03824300	-1.11074200
O	-3.22721300	0.58998000	0.94416900
C	-4.55772300	0.05902700	0.72704800
C	-5.46963000	0.37744600	1.89877700
H	-4.41666700	-1.01338300	0.61367100
H	-4.95102600	0.46074800	-0.21227700
H	-6.45752700	-0.06125300	1.73257000
H	-5.06122900	-0.03087600	2.82543200
H	-5.60134500	1.45696300	2.02250100
H	-3.26568400	1.55310400	1.01754200

U-M6-EtOH-cis

U	-1.12692500	-0.24140600	-0.09709600
O	-0.36416800	-0.27313000	1.50791500
O	0.62873200	1.39748200	-0.59191200
O	-1.81133100	-0.14891400	-1.72387700
O	-3.33490000	0.28085800	0.90786300
O	-2.91581200	-1.80988300	0.62236900
O	-4.83292000	-1.20488900	1.47794700
N	-3.75462100	-0.93267200	1.02733900
O	0.96137600	-1.28242600	-1.02506800
N	0.59242700	-2.51409300	-0.90797100
N	1.79335700	1.17817800	0.04216500
C	2.89857300	0.96209300	-0.62364700
N	2.88325700	1.11959000	-1.95743900
H	1.95970000	1.21823100	-2.36308500
H	3.57541700	0.62257200	-2.49489800
C	4.13227000	0.60147900	0.09588100
C	4.08906500	-0.34738700	1.12583800
C	5.35198500	1.19161700	-0.26072800
C	5.25655500	-0.68779100	1.80112700
H	3.15611700	-0.84309200	1.36700900
C	6.51380300	0.84399400	0.41916600
H	5.38193800	1.93403900	-1.04975000
C	6.46700300	-0.09308700	1.45061100
H	7.45466300	1.30800900	0.14809100
O	-0.57531400	-2.66121600	-0.41894800
O	1.30005200	-3.43137400	-1.23204600
H	5.22181000	-1.42926600	2.59014300
H	7.37498200	-0.36367600	1.97675000
H	1.76261500	1.08770700	1.05372500
O	-1.68389300	2.25665500	0.08768300

C	-2.83695300	3.01567900	-0.34005400
C	-2.84430400	4.39992200	0.28578300
H	-3.69426400	2.42968400	-0.01599100
H	-2.84599200	3.06781900	-1.43385800
H	-3.74451300	4.94270900	-0.01606800
H	-2.83429900	4.32773500	1.37530500
H	-1.97791600	4.98903600	-0.03151700
H	-0.85663700	2.65640900	-0.22098400

U-M2-M2

U	0.00001400	0.03484400	-0.00002900
O	0.92021100	0.04254400	1.51874000
O	1.50759900	-0.16587600	-3.03085400
O	-0.91996200	0.04312900	-1.51889400
O	0.91820300	2.30775400	-0.55709400
O	-0.91865500	2.30740200	0.55761500
O	-0.00041900	4.21132400	0.00052600
N	-0.00028800	3.01048200	0.00036200
O	0.93675800	-2.21929300	-0.52640900
N	-0.00013200	-2.92292100	-0.00122000
H	0.55020800	-0.05185500	-2.96277100
N	1.95857300	-0.00194200	-1.69620300
C	3.23704400	-0.22845000	-1.62866500
N	3.95076300	-0.65919600	-2.69663500
H	3.47573400	-0.72745400	-3.58290400
H	4.95121800	-0.56262800	-2.68589300
C	3.96121600	-0.04664900	-0.34776400
C	4.79256000	-1.07002100	0.12593900
C	3.85326400	1.14972200	0.36861000
C	5.50053600	-0.89888300	1.31059800
H	4.85836700	-2.00370400	-0.42039100
C	4.57000100	1.31500700	1.55057100
H	3.21435300	1.94073700	-0.00294800
C	5.39207400	0.29479100	2.02294000
H	4.48470100	2.24427100	2.10169600
O	-0.93674600	-2.21957600	0.52491400
O	-0.00037400	-4.12324700	-0.00198300
H	6.13023000	-1.69930000	1.68161500
H	5.94621100	0.42715200	2.94530200
N	-1.95827400	-0.00282100	1.69626100
O	-1.50688800	-0.16790000	3.03069000
C	-3.23672000	-0.22965800	1.62882400
N	-3.95001900	-0.66140600	2.69660600

H	-0.54966800	-0.05275100	2.96233600
H	-4.95053500	-0.56554500	2.68618800
C	-3.96115400	-0.04694700	0.34823300
C	-3.85353700	1.14999400	-0.36721000
C	-4.79240700	-1.07008400	-0.12615000
C	-4.57050800	1.31610000	-1.54891100
H	-3.21475200	1.94089300	0.00483200
C	-5.50061900	-0.89813300	-1.31056100
H	-4.85794100	-2.00423100	0.41941300
C	-5.39248900	0.29612400	-2.02196900
H	-4.48546800	2.24581400	-2.09931900
H	-6.13023800	-1.69838000	-1.68206700
H	-5.94679400	0.42914600	-2.94413300
H	-3.47464900	-0.73078800	3.58259700

U-M2-M2-cis

U	-0.00047600	-0.99170900	-0.00055200
O	-1.23177000	-0.91439300	1.27668500
O	0.19238300	1.67014800	-2.09241600
O	1.23095500	-0.91639600	-1.27778500
O	0.93189800	-3.12259900	0.88232700
O	1.73796200	-1.33701600	1.76240600
O	2.48486300	-3.28778400	2.41047300
N	1.75708900	-2.62683700	1.72279800
O	-0.93664200	-3.12048500	-0.88343200
N	-1.76290500	-2.62323100	-1.72208900
H	0.75689300	0.89853300	-2.23989800
N	-0.80193100	1.19542200	-1.19441600
C	-1.72672100	2.09624200	-1.04605200
N	-1.64098600	3.31996400	-1.63334700
H	-0.91449800	3.44574100	-2.32191700
H	-2.49133100	3.84644900	-1.74545500
C	-2.90673000	1.84629200	-0.18018100
C	-3.24089500	2.78528800	0.80537400
C	-3.71529900	0.72144400	-0.36990600
C	-4.36582800	2.59205900	1.59974400
H	-2.60387900	3.64782100	0.96008400
C	-4.84226500	0.53758000	0.42738100
H	-3.45929500	0.00082500	-1.13535200
C	-5.16896100	1.46781800	1.41083400
H	-5.46520000	-0.33620500	0.27650900
O	-1.74105300	-1.33353500	-1.76212500
O	-2.49382100	-3.28288300	-2.40764100
H	-4.61262500	3.31459700	2.36919800

H	-6.04595800	1.31804500	2.03020100
N	0.80422200	1.19366900	1.19450000
O	-0.18890600	1.66857900	2.09366500
C	1.73030900	2.09330700	1.04696200
N	1.64666300	3.31625400	1.63608500
H	-0.75520000	0.89787800	2.23936500
H	2.49753100	3.84186100	1.74813500
C	2.90971500	1.84266800	0.18052200
C	3.71520800	0.71506600	0.36715000
C	3.24655400	2.78346000	-0.80238400
C	4.84179900	0.53040800	-0.43043100
H	3.45695300	-0.00702400	1.13045100
C	4.37115900	2.58947000	-1.59706700
H	2.61184600	3.64808200	-0.95494300
C	5.17125500	1.46259400	-1.41114900
H	5.46233600	-0.34549100	-0.28195900
H	4.61999400	3.31351700	-2.36444400
H	6.04800900	1.31220900	-2.03071100
H	0.92038900	3.44244600	2.32477700

U-M1-M1-cis

U	-1.87391300	-0.10467500	-0.05889900
O	-2.15640900	-1.24288300	-1.37340900
O	-1.69186900	1.71509000	-1.73675400
O	-3.64532200	1.42153900	-0.89150000
O	-3.33783100	3.01589500	-2.35438800
N	-2.92509700	2.10334200	-1.69613100
O	-1.50701800	1.00618000	1.25859400
O	-2.53653700	-1.88657600	1.54855000
O	-4.12486400	-0.60556800	0.86796000
O	-4.58072700	-2.24931700	2.23219800
O	0.48476100	0.18876400	-0.97050500
N	-3.80118400	-1.61228100	1.58312700
H	0.80461900	-0.74548800	-1.01955700
O	-0.12180600	-1.92375300	0.81632400
N	0.97503500	-2.29686800	-0.07618700
C	2.08417000	-2.35232700	0.61431400
N	2.17975600	-2.12152000	1.93333800
C	3.31337800	-2.70007100	-0.14167000
H	3.04789400	-2.26103400	2.41840900
H	1.36610900	-1.79706400	2.43142500
C	4.51991000	-2.04639500	0.13542500
C	3.26524000	-3.67157500	-1.14751400
C	5.66818500	-2.37211800	-0.57957600

C	4.41730300	-3.99430200	-1.85666600
H	2.32660300	-4.16628200	-1.36119400
C	5.61951100	-3.34851300	-1.57259700
H	4.37685500	-4.75177700	-2.63059400
H	6.51544400	-3.60161400	-2.12774200
H	-0.69910400	-2.70144100	0.86615000
N	1.52646100	0.80144500	-0.15170400
C	1.69024100	2.04134300	-0.49111900
N	1.07932500	2.68978500	-1.51763600
C	2.69810800	2.79583100	0.30249600
H	0.27609200	2.24956900	-1.94834600
H	1.03183300	3.69432300	-1.45541800
C	3.52630700	3.73713800	-0.32070300
C	2.82825400	2.57047000	1.67765500
C	4.46953500	4.44192400	0.42201800
C	3.77155400	3.27824900	2.41551000
H	2.17551800	1.85087700	2.15435000
C	4.59357200	4.21526300	1.79092800
H	3.85772700	3.10713800	3.48260000
H	5.32478600	4.76857800	2.36918100
H	6.59708900	-1.85519200	-0.36910300
H	4.55054700	-1.25660700	0.87693400
H	3.44694500	3.89993500	-1.38927000
H	5.11031100	5.16439700	-0.07033600

U-M1-M1

U	0.01118200	0.01332100	0.01998400
O	1.03093600	0.04325300	-1.41567500
N	-3.37082600	-0.58226500	-0.99728900
O	0.93358200	-2.20720300	0.67212100
C	-4.11807400	0.42282500	-0.65857900
O	-2.06545400	-0.09893700	-1.48018300
O	-0.66805500	-2.28102800	-0.75430400
N	0.20394700	-2.94434000	-0.09645700
O	0.33922300	-4.13219700	-0.17757800
O	-1.00478700	-0.01280500	1.45674000
N	3.38624700	0.58838300	1.03551200
O	-0.90182000	2.23503100	-0.65177000
C	4.12469400	-0.43352300	0.73324400
O	2.07771300	0.13128300	1.53338200
O	0.69642100	2.31441600	0.77845000
N	-0.17504500	2.97482400	0.11769700
O	-0.31122100	4.16291100	0.19423700
H	1.87464600	0.82955600	2.17001700

H	-1.84796700	-0.78917700	-2.12088400
N	3.82329500	-1.74367500	0.92444600
H	2.87397300	-1.99639500	1.16717400
H	4.32242100	-2.41568500	0.36454600
C	5.46214700	-0.10202500	0.17071600
C	6.56893500	-0.90917100	0.46136100
C	5.62660400	1.02455000	-0.64325100
C	7.82035600	-0.59663100	-0.06153600
C	6.87949700	1.33213400	-1.16229200
H	4.76721500	1.64408800	-0.86321500
C	7.97791100	0.52286200	-0.87533900
H	6.99771000	2.20311600	-1.79654900
H	8.95276800	0.76468000	-1.28324500
N	-3.77076200	1.72877300	-0.64042200
H	-4.49168100	2.42344500	-0.55406800
H	-2.84302800	2.02946300	-0.90961400
C	-5.49319300	0.06322000	-0.21147200
C	-6.11413300	0.78198200	0.81678000
C	-6.17397900	-1.00074800	-0.81371400
C	-7.40105500	0.44675500	1.22859300
C	-7.45902000	-1.33177900	-0.39882100
H	-5.68608400	-1.55786300	-1.60269200
C	-8.07694700	-0.60812900	0.62016300
H	-7.98081200	-2.15462400	-0.87377800
H	-9.07929200	-0.86797600	0.94099200
H	8.67290100	-1.22318400	0.17416300
H	6.45657200	-1.76455300	1.11748100
H	-5.58063000	1.58214900	1.31691000
H	-7.87019000	1.00381900	2.03138000

U-M1-M2

U	0.37950800	0.30962000	-0.00475100
O	-0.40095100	0.92266200	1.46562100
O	-1.77230900	0.68894000	-1.45763800
O	1.18554300	-0.30476300	-1.44414100
O	1.89835600	2.31913500	-0.09651400
O	0.04796600	2.48788900	-1.16851400
O	1.47925500	4.13874000	-1.23191300
N	1.16755600	3.04598200	-0.85158900
O	0.58933000	-1.95559500	1.06315900
N	-0.49805100	-2.45248300	0.60018800
H	-1.60678900	1.57900600	-1.80266100
N	-3.04912900	0.85863200	-0.75746500

C	-3.81710000	-0.15470300	-1.00526000
N	-3.56111200	-1.15732700	-1.89584500
H	-2.60509000	-1.20292000	-2.21699600
H	-3.96312400	-2.05505100	-1.67219000
C	-5.12218200	-0.16867000	-0.29523300
C	-6.25235400	-0.72818700	-0.90401500
C	-5.23365700	0.38568900	0.98554000
C	-7.47427200	-0.73754100	-0.23765500
H	-6.17966300	-1.13163700	-1.90715700
C	-6.45730600	0.37492300	1.64556700
H	-4.35512100	0.81361200	1.45032900
C	-7.57913800	-0.18773600	1.03800200
H	-6.53447300	0.80131000	2.63916000
O	-1.17979200	-1.62979800	-0.11406400
O	-0.84995100	-3.58125700	0.80916100
H	-8.34557700	-1.16698800	-0.71873400
H	-8.53111800	-0.19697800	1.55664200
N	2.36591400	0.19308600	1.60621400
O	2.09729100	0.82780200	2.84645000
C	3.64833200	0.00449100	1.47539500
H	1.14070600	0.96702700	2.82912800
N	4.53637700	0.46706100	2.38301700
H	4.18100200	0.92247700	3.20890900
H	5.47598600	0.11066400	2.38056800
C	4.18337800	-0.71705900	0.29614000
C	3.69274800	-1.98040000	-0.04918100
C	5.22031800	-0.14307200	-0.45068600
C	4.23619300	-2.65866200	-1.13651200
H	2.89392200	-2.42310100	0.53217000
C	5.75281000	-0.82468200	-1.53960600
H	5.58461100	0.84466900	-0.19309600
C	5.26280100	-2.08419600	-1.88208600
H	3.85477900	-3.63811900	-1.40036200
H	6.54363100	-0.37006000	-2.12489200
H	5.67941200	-2.61481300	-2.73065000

U-M1-M2-cis

U	-1.41856400	-0.65483900	-0.10848900
O	-1.00996100	-1.81730400	-1.36614300
O	0.95181600	-1.38213100	1.02278000
O	-1.76394100	0.48547200	1.19067000
O	-3.67428700	-0.33347700	-1.06414800
O	-2.15880600	0.98681300	-1.83035600

O	-4.21480500	1.17214800	-2.55239300
N	-3.39972800	0.63416400	-1.85538100
O	-3.17239200	-2.24490100	0.74307300
N	-2.43086600	-2.92427400	1.52091400
H	0.69845400	-2.30421500	1.19535500
N	2.16894500	-1.45815800	0.23929300
C	3.13206000	-0.85367000	0.87312600
N	2.98689300	-0.20464000	2.05419900
H	2.09079700	-0.28983500	2.51147300
H	3.79924300	-0.05029800	2.62748400
C	4.46313900	-0.84489500	0.21515000
C	5.32917800	0.24436700	0.37388600
C	4.85837800	-1.92959000	-0.57741100
C	6.57532900	0.24378100	-0.24604100
H	5.01778100	1.10403000	0.95553300
C	6.10356700	-1.92359900	-1.19584800
H	4.18629000	-2.76951600	-0.69587400
C	6.96495500	-0.83985000	-1.03012700
H	6.40444100	-2.76861500	-1.80393200
O	-1.20655700	-2.50219000	1.56971100
O	-2.80907000	-3.86562100	2.16071100
H	7.23771100	1.09277500	-0.12309600
H	7.93596100	-0.83947500	-1.51177300
N	0.53244900	0.84702800	-0.87669400
O	1.30212200	0.17247400	-1.87175400
C	0.95222000	2.07418700	-0.73478900
H	1.63811000	-0.61666800	-1.39594900
N	2.05720900	2.53097800	-1.36803100
H	2.46029000	1.92476100	-2.06799300
H	2.19939800	3.52432300	-1.43394300
C	0.26660900	3.02578400	0.17910200
C	-1.06470900	3.39683700	-0.02539000
C	0.99653800	3.59601500	1.23016000
C	-1.65999400	4.32558100	0.82423100
H	-1.62227900	2.95992900	-0.84340400
C	0.39151900	4.51569600	2.08022500
H	2.02719200	3.30004000	1.38969100
C	-0.93795800	4.88257000	1.87654700
H	-2.69326600	4.60945300	0.66316700
H	0.95500900	4.94317700	2.90168200
H	-1.40947600	5.60009200	2.53832300

U-M6-M6

U	-0.02018500	0.15081200	-0.01989300
O	-1.00812000	-0.13291800	1.42650800
O	-1.89852600	-0.15997600	-1.40584900
O	1.03308500	0.42427400	-1.43692900
O	-0.54008600	-2.27566700	-0.68615400
O	1.25021000	-2.03778100	0.47317200
O	0.56541700	-4.04862000	-0.03967200
N	0.43716300	-2.84882200	-0.07870700
O	-1.46790100	2.22661100	-0.40359500
N	-0.76812200	3.05574700	0.28539800
N	-3.12901100	0.13882800	-0.98240000
C	-3.96840600	-0.81250300	-0.64560800
N	-3.54288500	-2.07978800	-0.65898200
H	-2.56063400	-2.27743900	-0.84786900
H	-4.20266900	-2.83278000	-0.57738300
C	-5.34523800	-0.46347800	-0.24887000
C	-6.04698300	0.54097300	-0.92838500
C	-5.95832200	-1.13312400	0.81855300
C	-7.33933800	0.87479700	-0.53713400
H	-5.59129500	1.04016900	-1.77543000
C	-7.25225600	-0.79728900	1.20086400
H	-5.40891800	-1.88945300	1.36693500
C	-7.94432700	0.20666500	0.52534700
H	-7.71616200	-1.31181700	2.03412500
O	0.30352100	2.55734700	0.76396200
O	-1.10055300	4.20286200	0.45435900
H	-7.87724900	1.65006000	-1.06981800
H	-8.95234500	0.46716300	0.82636800
H	-3.31469800	1.12227300	-0.79529700
O	2.01854700	0.45291000	1.15901000
N	3.15110800	0.40646800	0.45639100
C	4.27692700	0.05321000	1.02232900
H	3.06596500	0.52638600	-0.55266300
N	4.24042900	-0.33028700	2.31108800
C	5.52861600	0.04884600	0.24802200
H	3.33679500	-0.27092900	2.76372100
H	5.07769400	-0.29529100	2.86620500
C	5.78977000	1.05717300	-0.68987000
C	6.46805500	-0.97265000	0.44544900
C	6.96901700	1.03341400	-1.42672100
H	5.08621500	1.87095700	-0.82183200
C	7.64718200	-0.98555400	-0.29102000
H	6.25692700	-1.76849900	1.14992800
C	7.89908400	0.01482500	-1.22861200

H	7.16614400	1.81804300	-2.14748600
H	8.36456600	-1.78376600	-0.14111300
H	8.81845500	0.00101400	-1.80226600

U-M6-M6-cis

U	-0.00002200	0.58176900	-0.00012200
O	-0.96383300	0.56775700	-1.50106700
O	-1.31640700	-1.37971800	0.41956700
O	0.96381300	0.56875700	1.50077700
O	-2.07521500	0.97525200	1.40988000
O	-1.13104600	2.75803100	0.67158100
O	-2.95034600	2.92281600	1.86982800
N	-2.08992800	2.26083100	1.34159200
O	2.07581300	0.97486900	-1.41007400
N	2.09023700	2.26040700	-1.34173100
N	-2.54420600	-1.36902900	-0.11009500
C	-3.60994600	-1.49700600	0.63933300
N	-3.44867800	-1.68969500	1.95519100
H	-2.54245600	-1.44357900	2.33375300
H	-4.25433200	-1.67605700	2.55579100
C	-4.94928700	-1.43219200	0.02374700
C	-5.25906900	-2.20604900	-1.10062700
C	-5.91018400	-0.56420800	0.55931000
C	-6.52042300	-2.11188700	-1.68145500
H	-4.52294400	-2.89293900	-1.50185200
C	-7.16778300	-0.47627400	-0.02716300
H	-5.65371000	0.07030900	1.40017800
C	-7.47501300	-1.25034500	-1.14544200
H	-7.90309600	0.20705200	0.38077700
O	1.13047700	2.75741100	-0.67275100
O	2.95110900	2.92261900	-1.86891700
H	-6.75892700	-2.71700800	-2.54817100
H	-8.45617500	-1.17885200	-1.60022500
H	-2.62340800	-1.06419600	-1.07805400
O	1.31623900	-1.38000100	-0.41849700
N	2.54417700	-1.36918500	0.11073700
C	3.60973300	-1.49739200	-0.63888100
H	2.62369000	-1.06476600	1.07878600
N	3.44821400	-1.69047000	-1.95465500
C	4.94920300	-1.43233100	-0.02357300
H	2.54196400	-1.44427500	-2.33309100
H	4.25375000	-1.67629500	-2.55540200
C	5.25938200	-2.20619000	1.10069100

C	5.90979100	-0.56409300	-0.55926300
C	6.52082900	-2.11179000	1.68127700
H	4.52349600	-2.89328100	1.50201700
C	7.16748900	-0.47592100	0.02696800
H	5.65300200	0.07045700	-1.40001100
C	7.47512000	-1.24999900	1.14512900
H	6.75963500	-2.71691500	2.54790700
H	7.90256000	0.20760800	-0.38106800
H	8.45635500	-1.17831100	1.59972200

U-M2-M6

U	-0.31427200	0.11912500	-0.14628100
O	0.67233700	-0.12954500	1.32416700
O	1.59907800	0.58723700	-1.41385000
O	-1.33166400	0.36302800	-1.56536900
O	-0.97949100	-2.32551600	-0.06647100
O	0.87342900	-1.92588100	-1.07575000
O	0.19505800	-3.99128800	-0.85335400
N	0.03381200	-2.81222600	-0.67337100
O	-1.36980000	2.15718800	0.96215600
N	-0.49110300	3.02529100	0.63019200
N	2.77605600	0.04057600	-1.09336900
C	3.70962900	0.75058300	-0.51028300
N	3.47673600	2.05181300	-0.28175900
H	2.53294700	2.39849000	-0.44462300
H	4.04593800	2.52877000	0.39719300
C	4.99435200	0.12079400	-0.15318100
C	6.19389000	0.82076600	-0.33830300
C	5.02199700	-1.17504000	0.37941000
C	7.40496200	0.22625700	-0.00140200
H	6.17710900	1.81528600	-0.76878900
C	6.23799700	-1.76361400	0.71054700
H	4.09521200	-1.70677100	0.56170200
C	7.42919400	-1.06555200	0.52167400
H	6.25267000	-2.76348600	1.12753000
O	0.45409400	2.55043000	-0.09880800
O	-0.54025300	4.17940500	0.96876600
H	8.33039700	0.76866200	-0.15481200
H	8.37445400	-1.52619800	0.78391700
N	-2.20790900	-0.47196500	1.54760600
O	-1.66936800	-0.90925600	2.78526500
C	-3.47067700	-0.77019900	1.48092500
H	-0.73102300	-0.68764600	2.70949400

N	-4.09394000	-1.49600200	2.44365400
H	-3.56420000	-1.72254300	3.27074700
H	-5.09611000	-1.45083000	2.50971100
C	-4.27826200	-0.34448000	0.31297700
C	-4.25761900	0.98429300	-0.12311000
C	-5.09814900	-1.27730500	-0.33568100
C	-5.04664700	1.36996200	-1.20296500
H	-3.62925300	1.70551100	0.38383800
C	-5.87996500	-0.88464400	-1.41664900
H	-5.09703100	-2.31063700	-0.00879000
C	-5.85610600	0.43999400	-1.85073300
H	-5.02575700	2.40019800	-1.53859100
H	-6.49958600	-1.61376600	-1.92596100
H	-6.46496100	0.74464000	-2.69448100
H	2.90169800	-0.93885800	-1.33430200

U-M2-M6-cis

U	0.73727700	-0.97338800	0.03193800
O	1.85571300	-0.68466700	-1.30032700
O	-0.52756400	1.64177200	1.86563800
O	-0.40399500	-1.16152900	1.39564400
O	0.67109800	-3.46048900	-0.40862100
O	-0.76278500	-2.30356300	-1.50568500
O	-0.73116600	-4.47866200	-1.74035700
N	-0.29036400	-3.47699500	-1.24139200
O	2.45907000	-2.39106300	1.18143200
N	3.02831700	-1.46640600	1.85081000
H	-0.56129400	0.73575800	2.21108800
N	0.59084800	1.57969100	0.96707600
C	0.99360500	2.77738900	0.68007800
N	0.36627700	3.89638600	1.14974500
H	-0.28146000	3.75426100	1.91076100
H	0.90872600	4.74493400	1.17062700
C	2.13703600	2.97354400	-0.24423700
C	2.03755400	3.92964300	-1.26449200
C	3.31946400	2.24248700	-0.09007900
C	3.10771100	4.14344300	-2.12642900
H	1.11479900	4.48291800	-1.39602900
C	4.38677300	2.46607800	-0.95521900
H	3.39861800	1.51156800	0.70422800
C	4.28447500	3.41237600	-1.97202700
H	5.30007200	1.89599200	-0.83236200
O	2.49549100	-0.30169000	1.68825100

O	3.97348200	-1.65031200	2.56999700
H	3.01980500	4.87303100	-2.92321600
H	5.11778100	3.57820600	-2.64529700
N	-2.06717700	0.68163800	-0.47307500
O	-0.91895800	0.29883700	-1.04289000
C	-3.21613100	0.15252600	-0.81625700
N	-3.24921300	-0.78361100	-1.77611300
H	-2.36367000	-1.21312800	-2.04146700
H	-4.06993300	-1.36459000	-1.83137000
C	-4.45714800	0.63561300	-0.17755200
C	-4.49540000	0.89755300	1.19810400
C	-5.61014100	0.82572600	-0.95069000
C	-5.66990200	1.35448800	1.78702600
H	-3.61990500	0.71403400	1.80965700
C	-6.78113000	1.28071500	-0.35415000
H	-5.57953700	0.64143300	-2.01824300
C	-6.81285700	1.54702200	1.01359200
H	-5.69550900	1.54612900	2.85315000
H	-7.66719800	1.43335200	-0.95888300
H	-7.72736200	1.89935200	1.47616500
H	-2.00074900	1.40280200	0.24289000

U-M5-M5-NO3

U	-0.00230400	-0.94300900	-0.13214400
O	-0.87778900	-1.02864100	1.37876000
O	0.87417100	-0.83618400	-1.64085400
O	-0.01890600	-3.34353300	-0.33916000
H	0.46106100	-3.75420600	-1.07404600
C	-0.70800000	-4.42284100	0.44229400
C	0.25991600	-5.51537000	0.82781000
H	-1.51898600	-4.78756700	-0.18923100
H	-1.12606800	-3.90273200	1.30221700
H	-0.28296700	-6.28181700	1.38733500
H	0.69353300	-6.00414300	-0.04910700
H	1.06243400	-5.14322800	1.46764200
O	-2.13669200	-1.22727000	-1.38170200
N	-3.27385900	-0.39721600	-1.02162800
C	-2.87045500	0.78227700	-0.71526400
N	-1.46874700	1.13154700	-0.87790700
C	-3.81388300	1.76347500	-0.17992600
H	-1.30897300	2.05266500	-0.47576000
C	-3.62788000	3.13839300	-0.41347700
C	-4.93960200	1.32486000	0.53970600

C	-4.55252000	4.05509000	0.06841500
H	-2.79764200	3.50134000	-1.01124100
C	-5.85620800	2.24995900	1.01850100
H	-5.07857000	0.26779300	0.72568900
C	-5.66458900	3.61262500	0.78604700
H	-4.41566600	5.11167300	-0.12527800
H	-6.71922000	1.91105600	1.57802700
H	-6.38277900	4.33108400	1.16245900
N	3.28129500	-0.59386800	0.81554200
C	2.90343200	0.62558000	0.68364900
O	2.12757600	-1.44388000	1.05476500
N	1.50869600	0.97772600	0.89472400
C	3.86970800	1.65349600	0.29725400
C	4.98819900	1.30001800	-0.47834200
C	3.71338500	2.98284500	0.73060800
C	5.92747600	2.26441500	-0.81417900
H	5.10405200	0.27912900	-0.81841000
C	4.66064700	3.93913500	0.39059500
H	2.88862000	3.27240400	1.37422800
C	5.76581000	3.58177500	-0.38296000
H	6.78498800	1.99219400	-1.41693200
H	4.54681400	4.95845400	0.73790100
H	6.50194300	4.33103300	-0.64822300
H	-1.24854900	1.19393900	-1.87546900
H	1.36963800	1.94883100	0.62389600
H	-2.53362900	-1.96969100	-1.85764000
H	2.51304300	-2.26340200	1.39370000
H	1.28770100	0.90635000	1.89150000

U-M5-M5-NO3'

U	-0.00176400	0.04008200	0.05351900
O	0.71618200	-0.18051400	1.63425700
O	-0.71682400	0.39252600	-1.50435700
O	0.00162300	2.40637700	0.52675700
H	0.36887300	2.70609000	1.37160900
C	-0.50586400	3.60077800	-0.22140500
C	0.56447400	4.65826600	-0.34860700
H	-1.37932500	3.95780700	0.32584400
H	-0.82123200	3.19841300	-1.18221600
H	0.15157200	5.51117200	-0.89377100
H	0.89042000	5.02785600	0.62759800
H	1.43071000	4.29552600	-0.90538100
O	-1.32149400	-2.03275400	0.37397000

N	-2.75590000	-2.03248500	0.13317400	C	-2.61662400	4.40721300	-1.43644900
C	-3.25334200	-0.89454800	0.46161800	H	-0.45812400	4.65144900	-1.37746500
N	-2.41602200	0.10102400	1.11128700	H	-1.17818100	4.20868000	0.18721600
C	-4.65484800	-0.59927400	0.16807500	H	-2.81508000	5.46845700	-1.26431500
H	-2.90799400	0.99211500	1.13246200	H	-2.67695000	4.23977800	-2.51545000
C	-5.38559200	0.29052300	0.97695600	H	-3.40230100	3.83634400	-0.93773300
C	-5.29086600	-1.24523500	-0.90766500	O	2.11446500	1.96300300	-0.37602900
C	-6.72733700	0.52751600	0.71117900	N	3.24333600	1.12105700	-0.73397700
H	-4.93475800	0.76603500	1.84211200	C	3.26149600	0.07305200	0.00727900
C	-6.63184700	-1.00003400	-1.16470000	N	2.30802100	-0.05632500	1.09909600
H	-4.72693600	-1.92217700	-1.53613400	C	4.22770600	-0.99243700	-0.25647000
C	-7.35047600	-0.11522800	-0.35934000	H	2.32812400	-1.01426700	1.44389900
H	-7.29128300	1.20195600	1.34337700	C	4.68455200	-1.82031100	0.78531500
H	-7.11845000	-1.49379200	-1.99664800	C	4.73706100	-1.16397700	-1.55643300
H	-8.39722100	0.07378200	-0.56498700	C	5.63278000	-2.80107900	0.52781200
N	2.74121500	-1.89390900	-0.71856700	H	4.34539800	-1.68081500	1.80661900
C	3.24772700	-0.71775000	-0.61628200	C	5.68347400	-2.14774200	-1.80260800
O	1.31178300	-1.79579200	-0.97090800	H	4.37925700	-0.53389500	-2.36027800
N	2.42631600	0.45059200	-0.88987500	C	6.13124100	-2.96669600	-0.76479400
C	4.64306200	-0.55863100	-0.20996700	H	5.99195000	-3.42845200	1.33398600
H	2.92059500	1.28803500	-0.58833700	H	6.07008600	-2.28234300	-2.80517400
C	5.25086700	-1.54401500	0.58909900	H	6.86942000	-3.73453200	-0.96273200
C	5.39614200	0.54689800	-0.64653900	N	-1.72239700	-1.85949800	1.42295600
C	6.58630700	-1.41852600	0.94299100	C	-2.61409800	-1.22565300	0.74758300
H	4.66949200	-2.38961100	0.93287700	O	-0.68383300	-0.93010100	1.86028000
C	6.73231400	0.66115000	-0.28807600	N	-2.55039500	0.21988300	0.64111400
H	4.96688900	1.29730000	-1.30258200	C	-3.67643500	-1.96847900	0.07165800
C	7.32732500	-0.31895400	0.50751400	H	-3.23024500	0.54209500	-0.04450100
H	7.05109700	-2.17481000	1.56323200	C	-3.44667800	-3.29487800	-0.33653500
H	7.31390900	1.50540000	-0.63670900	C	-4.93963800	-1.38392100	-0.13523600
H	8.36968500	-0.22511300	0.78741500	C	-4.46473100	-4.01615300	-0.94297700
H	2.28064900	0.52982200	-1.89950400	H	-2.47245700	-3.74126600	-0.18567100
H	-2.25336300	-0.17855400	2.08206100	C	-5.95156800	-2.11573500	-0.74121900
H	-1.09999100	-2.96614100	0.49922200	H	-5.15975100	-0.37994400	0.21316300
H	1.09124600	-2.62155500	-1.42423400	C	-5.71476100	-3.42982900	-1.14694200
				H	-4.28475100	-5.03493300	-1.26295900
				H	-6.92699500	-1.66888200	-0.88751100
				H	-6.50613300	-3.99705300	-1.62201400
				H	2.59791400	0.55186000	1.86948000
				H	-2.79739800	0.63953900	1.54067300
				H	2.34193500	2.82399200	-0.75292400
				H	-0.34963600	-1.32504200	2.67717900
U-M5-M5-NO3''							
U	-0.02231300	0.91181500	0.32745700				
O	0.01734700	-0.15801000	-1.05383800				
O	-0.11572400	2.01570100	1.68290500				
O	-0.91421000	2.63230700	-1.10698200				
H	-1.02334500	2.42996400	-2.04823100				
C	-1.24781900	4.07716700	-0.89103300				

U-M7-M7-NO3

U	-0.02027400	0.83229200	0.14120600
O	-0.21166300	0.04690300	-1.42187100
O	0.00577700	1.65457700	1.69983000
O	-1.03494500	2.80736900	-0.83903900
H	-1.21885800	2.79172800	-1.78893200
C	-1.08706400	4.21892500	-0.36644300
C	-2.38240700	4.88052900	-0.77604600
H	-0.21252300	4.72209500	-0.78116100
H	-0.97599900	4.14493600	0.71382300
H	-2.38709700	5.90966400	-0.40799100
H	-2.48781300	4.92651700	-1.86375200
H	-3.24926700	4.36824500	-0.35409100
O	2.03605600	1.67150200	-0.47312700
N	3.15462400	0.95357000	-0.56874700
C	3.35196700	-0.12544100	0.14537300
N	2.33817400	-0.35591500	1.09490400
C	4.48149700	-1.00873400	-0.07034300
H	2.33958200	-1.30349500	1.45910700
C	5.02984600	-1.71966400	1.01543900
C	5.05404100	-1.14134600	-1.35190100
C	6.14014200	-2.52829400	0.82230400
H	4.61921900	-1.60986000	2.01265300
C	6.16248200	-1.95428900	-1.53245500
H	4.60730500	-0.65168100	-2.21010900
C	6.70795700	-2.64444300	-0.44764500
H	6.57038800	-3.06150100	1.66078300
H	6.59423700	-2.06534100	-2.51925600
H	7.57316800	-3.27976000	-0.59425300
N	-1.66878700	-1.84970000	0.80150200
C	-2.78692100	-1.20617600	0.58853300
O	-0.53703200	-1.21963000	1.13881900
N	-2.70624000	0.17340000	0.84163400
C	-3.97936000	-1.86110700	0.08188100
H	-3.54045200	0.67306600	0.55262600
C	-3.87097100	-2.95358200	-0.80123200
C	-5.25187400	-1.41816600	0.49234500
C	-5.01590400	-3.59561500	-1.24905900
H	-2.90224100	-3.26508400	-1.17547700
C	-6.38936200	-2.07111500	0.04025700
H	-5.35438200	-0.59926300	1.19575700
C	-6.27314400	-3.15831500	-0.82765000
H	-4.93308300	-4.42601200	-1.93906600

H	-7.36655700	-1.74067700	0.36947600
H	-7.16469200	-3.66166600	-1.18185500
H	2.37207400	0.31235900	1.86721000
H	-2.48798900	0.37855600	1.81862000
H	3.86185800	1.31777800	-1.20334600
H	-1.62714500	-2.86567800	0.77621000

U-M6-M6-NO3

U	-0.00125500	0.91131800	0.15300700
O	0.77044900	0.74544300	1.73130400
O	-0.76811400	1.13338100	-1.42022800
O	0.04564500	3.31384600	0.47728800
H	0.42411000	3.66250100	1.29696800
C	-0.43931800	4.45671800	-0.34896400
C	0.66183500	5.46513500	-0.57968800
H	-1.29357600	4.88239800	0.17926700
H	-0.78277500	3.99235400	-1.27158200
H	0.27077100	6.28230300	-1.19133200
H	1.01257100	5.90343200	0.35888700
H	1.50874400	5.02334800	-1.10818100
O	-1.79085600	-0.23973400	0.78588500
N	-2.95954100	-0.58672500	0.18728600
C	-3.88655400	-1.25247300	0.86468200
N	-3.63461600	-1.60737700	2.11638900
C	-5.15355800	-1.58375600	0.20243900
H	-4.36891800	-1.98686600	2.69373700
C	-5.75072000	-2.83322800	0.43481700
C	-5.76784700	-0.65967600	-0.65813700
C	-6.94707500	-3.15176500	-0.19496800
H	-5.26755000	-3.56451900	1.07263100
C	-6.96631600	-0.98838500	-1.27919300
H	-5.34127200	0.32617800	-0.80492100
C	-7.55435800	-2.23217400	-1.05015700
H	-7.40270300	-4.11925000	-0.02452500
H	-7.44984400	-0.27035800	-1.92979900
H	-8.48958500	-2.48385100	-1.53549400
N	2.93275100	-0.57377300	-0.19970400
C	3.85742500	-1.10365100	-0.99014900
O	1.77654700	-0.09069800	-0.72507400
N	3.61461200	-1.19505900	-2.28978700
C	5.11318800	-1.58091700	-0.39904400
H	4.35038900	-1.46132000	-2.92557700
C	5.73543500	-0.85530400	0.62955400

C	5.69261000	-2.76941000	-0.87161100
C	6.92478100	-1.31980500	1.17744900
H	5.32281700	0.08900800	0.96637000
C	6.87966600	-3.22575500	-0.31295700
H	5.20271500	-3.35193500	-1.64341500
C	7.49529400	-2.50315800	0.70911900
H	7.41480300	-0.75238700	1.95885800
H	7.32153000	-4.14793200	-0.66933300
H	8.42328900	-2.86084600	1.13859500
H	2.72357600	-0.89418700	-2.65956200
H	-2.73592100	-1.39942300	2.52910800
H	-3.04669900	-0.42328400	-0.80969300
H	3.01022200	-0.61837700	0.81054100

U-M9

U	-1.02666000	-0.00907000	0.01961000
O	-1.03640700	0.08002100	-1.75531400
O	0.51602300	1.98207500	0.04011900
O	-1.58205500	2.49191600	0.06176100
O	-0.08636100	4.08031200	0.02166100
N	-0.37868100	2.90462900	0.04021400
O	-1.04535300	-0.01753200	1.79535300
O	-2.80438300	-1.80696600	-0.03487100
O	-3.53361700	0.22538500	0.01782400
O	-4.95497900	-1.43085600	-0.03204700
N	-3.81410400	-1.02317400	-0.01697200
O	0.12755800	-2.00451100	-0.06271700
N	1.15814700	-1.12631900	-0.01059900
C	2.35151200	-1.62206700	-0.06615100
N	2.52886000	-3.00282300	-0.09124700
C	3.53972500	-0.74921600	-0.03671600
H	3.24730100	-3.31607300	-0.72961800
H	1.63457800	-3.46024200	-0.23865200
C	4.79816400	-1.28687300	0.27547900
C	3.44464400	0.62340600	-0.31750400
C	5.93284600	-0.47946100	0.29422500
C	4.57940900	1.42422200	-0.28769000
H	2.48265600	1.06233200	-0.54414700
C	5.82955900	0.87961300	0.01099000
H	4.48283100	2.48340700	-0.49965100
H	6.71159100	1.51105400	0.02873100
H	4.87971700	-2.33523800	0.53680100
H	6.89586700	-0.91345700	0.54273500

U-M10

U	1.02728600	-0.06300100	-0.00068300
O	1.00717200	-0.00663100	-1.77737300
O	2.21837600	-2.29185400	0.00016300
O	3.50993300	-0.56583000	0.00188200
O	4.38527200	-2.56639500	0.00292000
N	3.41516600	-1.84106700	0.00171000
O	1.00360800	-0.00740300	1.77597300
O	0.42836700	2.41947800	-0.00112400
O	2.54479500	2.01443500	0.00205600
O	1.84447500	4.08102200	0.00232000
N	1.62532300	2.88901300	0.00115200
O	-0.57658300	-1.71000400	-0.00204300
N	-1.89482300	-1.65093800	-0.00109900
C	-2.41474000	-0.46674100	-0.00096200
N	-1.51891300	0.67008100	-0.00190500
C	-3.87258600	-0.29469500	-0.00001300
H	-1.64145500	1.26670200	0.81301000
H	-1.64203200	1.26569600	-0.81747700
C	-4.45992500	0.98110300	-0.00043200
C	-4.73001400	-1.41402500	0.00130300
C	-5.84558700	1.13529600	0.00038800
C	-6.10677000	-1.25432100	0.00211800
H	-4.28365500	-2.39986500	0.00165700
C	-6.67846500	0.02190200	0.00166500
H	-6.74472500	-2.13232300	0.00314200
H	-7.75645500	0.14128700	0.00229600
H	-3.83352600	1.86560400	-0.00140400
H	-6.27050000	2.13373100	0.00002400

U-M8

U	1.28401300	-0.03807000	0.12089100
O	1.99409200	0.30390200	1.71389800
O	0.45395900	2.34096700	-0.00062900
O	2.43891300	2.03625200	-0.79900300
O	1.55959300	4.03308500	-0.82562700
N	1.49295000	2.85542800	-0.55565900
O	0.65034300	-0.35908500	-1.50601700
O	2.09562800	-2.40412300	0.28994800
O	3.50855500	-1.02560700	-0.59568700
O	4.05231100	-3.12493200	-0.35410300
O	-0.68345800	-0.36407400	0.98134600
N	3.25575400	-2.22325300	-0.22659200

N	-1.93520300	-0.78097800	0.61648900
C	-2.79212500	0.18220800	0.50247700
N	-2.52664600	1.51606900	0.78291400
C	-4.17557800	-0.18275200	0.11846500
H	-1.53936800	1.70380900	0.90779600
H	-2.95192300	2.16906300	0.13941500
C	-5.24962100	0.67403900	0.39645000
C	-4.43819600	-1.39963200	-0.53008600
C	-6.54940000	0.32755300	0.03158400
C	-5.73543600	-1.74369700	-0.88674700
H	-3.60573200	-2.05791300	-0.74170500
C	-6.79903700	-0.88103700	-0.61191000
H	-5.91959000	-2.68747000	-1.38942900
H	-7.81032000	-1.15078500	-0.89750500
H	-5.06527900	1.60134200	0.92569400
H	-7.36811600	1.00239400	0.25928700

U-M8-M1-cis

U	-1.48136800	-0.69392100	-0.04927000
O	-1.04227200	-1.81491900	-1.35140000
O	-2.54609500	0.85688800	-1.76373500
O	-3.89730600	-0.58017600	-0.91169800
O	-4.64987100	0.87445800	-2.35628400
N	-3.74553800	0.40025700	-1.70424700
O	-1.95307900	0.37381600	1.28723300
O	-1.18508800	-2.53009600	1.70422000
O	-3.15611400	-2.47766400	0.85290100
O	-2.69659000	-3.94100200	2.40543300
O	0.02821900	0.78547700	-0.66927500
N	-2.37335400	-3.02512400	1.68270400
O	1.00423000	-1.20495200	1.36072000
N	2.09741400	-1.93407500	0.79024600
C	3.02136100	-1.12968900	0.37887300
N	3.01919600	0.22767900	0.48488100
C	4.21495900	-1.79348500	-0.22131300
H	3.75395700	0.72494300	0.01193500
H	2.13415200	0.73541000	0.54365900
C	4.93230200	-1.18920000	-1.26022100
C	4.63154000	-3.04867000	0.24110400
C	6.04427800	-1.81761500	-1.81689200
C	5.74051200	-3.67487000	-0.31559400
H	4.06538700	-3.51861800	1.03454600
C	6.45534900	-3.06074200	-1.34438700

H	6.05048100	-4.64578300	0.05599600
H	7.32140800	-3.55035500	-1.77666500
H	0.55623400	-1.89375000	1.87212200
N	0.63200800	1.83534100	-0.02911400
C	0.22289300	3.00445500	-0.40759100
N	-0.69563400	3.21951300	-1.41677200
C	0.84959500	4.18579800	0.23057600
H	-1.18617400	2.38123500	-1.71241600
H	-1.31962000	3.99813800	-1.26054800
C	0.89934800	5.41840100	-0.43553300
C	1.40441000	4.09411600	1.51647600
C	1.48849500	6.52851200	0.16606300
C	1.99694900	5.20182100	2.11015000
H	1.35413500	3.14576000	2.03575600
C	2.04015000	6.42600200	1.44033400
H	2.41791500	5.11367500	3.10615100
H	2.49699300	7.29064100	1.90994100
H	6.58123000	-1.33798200	-2.62822000
H	4.60220800	-0.23890000	-1.66504000
H	0.49604500	5.49454200	-1.43836300
H	1.52176400	7.47298300	-0.36708600

U-M8-M1

U	0.53354900	-0.19202200	-0.09246900
O	-0.25149500	0.13823300	-1.65045200
O	1.20426200	2.25818400	0.05903600
O	-0.73492600	1.81099500	0.88883300
O	-0.00013900	3.86690600	0.91168700
N	0.15066100	2.70129300	0.63211800
O	1.22378800	-0.49876400	1.51220100
O	0.06106400	-2.64861800	-0.42765100
O	-1.50899800	-1.55807300	0.57992100
O	-1.78918400	-3.67191500	0.11735900
O	2.48998400	-0.32322400	-0.99730500
N	-1.10568200	-2.67269300	0.09047700
O	-3.20040100	0.84293500	1.68329800
N	-4.40038400	1.13605700	1.00693900
C	-5.02589300	0.04144100	0.72981900
N	-4.58005200	-1.21966100	1.07928500
C	-6.33872100	0.16395500	0.04920500
H	-4.81615700	-1.94342800	0.41494100
H	-3.59061700	-1.23500000	1.31138700
C	-7.28135100	-0.87004200	0.11561200
C	-6.66091700	1.32192100	-0.67394500

C	-8.51059200	-0.75404200	-0.53129100
C	-7.88808300	1.43592300	-1.31418500
H	-5.93108500	2.11965300	-0.71965300
C	-8.81917300	0.39721000	-1.24960700
H	-8.11859700	2.33642400	-1.87367800
H	-9.77477700	0.48705300	-1.75511500
H	-2.63431700	1.61155600	1.52812100
N	3.78143600	-0.65848600	-0.68542000
C	4.57725400	0.35986700	-0.61553300
N	4.21272000	1.66884800	-0.89309800
C	5.99666000	0.08930100	-0.28733500
H	3.21140000	1.79371400	-0.97520500
H	4.63252000	2.35888400	-0.28624600
C	7.00123100	1.00513700	-0.62860200
C	6.36212100	-1.09526000	0.37047300
C	8.33469800	0.74701300	-0.31626500
C	7.69274400	-1.35116500	0.67493000
H	5.58311800	-1.79953200	0.63179200
C	8.68689800	-0.43040700	0.33713800
H	7.95724200	-2.27099300	1.18585800
H	9.72451600	-0.63121400	0.58183900
H	-9.22910800	-1.56434800	-0.46621500
H	-7.06008200	-1.75694200	0.69752700
H	6.73666400	1.90846400	-1.16540200
H	9.09896200	1.46584700	-0.59283500

U-M8-M2-cis

U	1.26126300	-0.75008000	-0.02446300
O	1.82122800	0.04595100	-1.51191800
O	-0.46199300	0.74517900	2.63201600
O	0.73943400	-1.49884500	1.52025000
O	2.78020000	0.89199300	1.23824000
O	3.74474200	-0.94626000	0.67081500
O	4.91034800	0.62290300	1.64168500
N	3.86184300	0.20142400	1.20012800
O	0.45996600	-2.77116700	-1.33955400
N	1.53870000	-3.45019800	-1.26610700
H	-0.18881100	-0.18422100	2.54574400
N	0.02552800	1.30966700	1.43738100
C	-0.46183500	2.48971900	1.25712000
N	-1.43027000	3.03057700	2.07927900
H	-1.60027100	2.48896900	2.91454300
H	-1.38822700	4.02910100	2.20966000
C	-0.03295500	3.29627700	0.09082000

C	-0.98280000	4.04263500	-0.62103300
C	1.31011100	3.33823500	-0.30116500
C	-0.59347900	4.81864300	-1.70815700
H	-2.02636800	3.97872600	-0.33772600
C	1.69063700	4.11434600	-1.39247900
H	2.04511500	2.76542700	0.25070500
C	0.74516800	4.85784500	-2.09573300
H	2.73197500	4.13281700	-1.69349200
O	2.48630100	-2.87942200	-0.62544300
O	1.65769000	-4.54875800	-1.76479500
H	-1.33785200	5.38114300	-2.26181700
H	1.04799700	5.45923800	-2.94645000
N	-1.99091000	-0.79388800	-0.10304400
O	-0.82018300	-0.39249000	-0.68684600
C	-3.02572300	-0.25688200	-0.66677800
N	-2.92993600	0.70539900	-1.67279600
H	-3.58367700	0.57040600	-2.43293700
C	-4.36591800	-0.63364300	-0.17431100
C	-4.54617900	-1.80760600	0.57573100
C	-5.48629400	0.16389000	-0.44888000
C	-5.80721400	-2.16670600	1.03191700
H	-3.67857400	-2.42014400	0.78423600
C	-6.75148800	-0.20421800	0.00548300
H	-5.35682100	1.08947000	-0.99735300
C	-6.91930500	-1.37039000	0.74642000
H	-5.92766400	-3.07812600	1.60827600
H	-7.60555700	0.42837100	-0.21430300
H	-7.90393900	-1.65826900	1.09955800
H	-1.96641300	0.75806300	-1.99123500

U-M8-M2

U	-0.20078600	-0.08061200	-0.09765400
O	-0.94952600	0.33226100	-1.65750600
O	-2.03754500	-0.52326300	2.85215000
O	0.39294500	-0.45991600	1.55930100
O	-1.23954500	2.16664900	0.79057700
O	0.74750400	2.33221300	-0.00700800
O	-0.29419100	4.13185900	0.66148100
N	-0.26439100	2.93065500	0.48854400
O	-1.63664900	-2.19225400	-0.07829500
N	-0.80019900	-2.95804200	-0.67285700
H	-1.07275500	-0.54510300	2.72583800
N	-2.49469100	-0.19307700	1.56008900
C	-3.78096200	-0.25824200	1.50214400

N	-4.54967700	-0.71774100	2.55470300	O	-2.36647400	-2.97299600	-0.88161100
H	-4.03053400	-0.82184900	3.41493000	O	-4.28543900	-2.34890200	-1.71331500
H	-5.45667600	-0.28768300	2.64937300	O	1.10122400	-0.06096300	0.88226400
C	-4.49084400	0.10922000	0.25532600	N	-3.16771900	-2.08637300	-1.30997600
C	-5.59964900	-0.64302600	-0.15695900	O	-0.61147500	0.71018000	-1.16112200
C	-4.08689500	1.21150500	-0.50665500	N	-1.57402400	1.52075600	-0.74146900
C	-6.28781600	-0.30281900	-1.31697200	C	-1.29433300	2.63484100	-0.10663700
H	-5.89639800	-1.51086900	0.42009400	N	-0.01381000	2.94274200	0.14056000
C	-4.77826500	1.54351400	-1.66813100	C	-2.40071600	3.52089200	0.30813300
H	-3.24112600	1.80334000	-0.18065200	H	0.18642700	3.80289500	0.61912900
C	-5.87831100	0.79216300	-2.07614300	H	0.73037300	2.21537100	0.08414300
H	-4.45023200	2.39303000	-2.25635100	C	-2.36372000	4.15439900	1.55811600
O	0.31122500	-2.40732700	-0.96554200	C	-3.50158300	3.73694700	-0.53210200
O	-1.04965100	-4.11591000	-0.93140100	C	-3.40753000	4.98124400	1.95870400
H	-7.13414500	-0.90165000	-1.63618300	C	-4.54656400	4.55960500	-0.12346500
H	-6.41018400	1.05403100	-2.98468800	H	-3.52663800	3.27450400	-1.51170800
N	3.07673300	-0.49622600	-0.55426900	C	-4.50218200	5.18624300	1.12023300
O	1.82043800	-0.06477000	-0.85830500	H	-5.39244000	4.71790400	-0.78282700
C	3.94721900	0.46112300	-0.49323600	H	-5.31641100	5.82910500	1.43547400
N	3.67228500	1.79382200	-0.76829500	N	1.95112400	0.85943600	0.35477900
H	4.15167100	2.44605600	-0.16301000	C	3.20300200	0.52900800	0.42430500
C	5.34538700	0.08685500	-0.18104500	N	3.64472900	-0.62628600	1.05038600
C	5.63580600	-1.14174500	0.43387300	C	4.20568300	1.47272300	-0.11136300
C	6.40827500	0.94634900	-0.49294800	H	2.87721500	-1.24832400	1.29376800
C	6.94692200	-1.49184900	0.72766800	H	4.39376100	-1.10447900	0.56891000
H	4.81252800	-1.80402600	0.66804000	C	5.51841300	1.48194900	0.38280500
C	7.72257100	0.59339700	-0.19124500	C	3.86867500	2.37463300	-1.13411100
H	6.20328500	1.88142900	-1.00061300	C	6.46369900	2.37135200	-0.12347200
C	7.99906700	-0.62522900	0.42138200	C	4.81254900	3.26506800	-1.63074500
H	7.15174900	-2.44488700	1.20439300	H	2.86304900	2.35042900	-1.53489100
H	8.53128500	1.27123300	-0.44489000	C	6.11640000	3.26851200	-1.13040300
H	9.02166500	-0.90042800	0.65748300	H	4.53527800	3.95114000	-2.42450200
H	2.67665600	1.98434900	-0.81095700	H	6.85323600	3.95901400	-1.52706000

U-M8-M6-cis

U	-0.42447000	-1.44272900	-0.06533200
O	-1.45050900	-1.08714000	1.34626400
O	1.31347200	-2.75004400	1.31251700
O	-0.30826100	-3.95737200	0.58099700
O	1.33102000	-4.90646500	1.66719600
N	0.79725500	-3.91791000	1.20389600
O	0.55768300	-1.83998300	-1.49279100
O	-2.71492000	-0.89200500	-1.29599900

U-M8-M6

U	-0.08792100	0.70655700	0.16310800
O	0.96079000	0.22145200	-1.20258300
O	-0.18150900	-1.70544700	0.77882000
O	1.70145400	-2.82592200	0.68730900

O	-0.16771700	-3.77254800	0.13623000
N	0.45507100	-2.79019100	0.51661200
O	-1.02548700	1.20379400	1.58989000
O	-0.41583700	2.97294500	-0.99360600
O	1.31140200	2.88403400	0.29228300
O	0.94659700	4.67641800	-0.90296200
O	-1.91291000	0.18316100	-0.89035100
N	0.62186300	3.55994400	-0.55426800
O	1.84208700	0.44319800	1.54995200
N	2.82472000	-0.33011100	1.08232300
C	3.88705200	0.19189300	0.53463400
N	4.02151900	1.54224700	0.52453000
C	4.94784800	-0.67671700	-0.01099500
H	4.58157200	1.92257800	-0.22211800
H	3.16667600	2.06119500	0.72509900
C	6.28311300	-0.25056600	0.02807100
C	4.64023000	-1.91925300	-0.58503300
C	7.29319300	-1.05161600	-0.49450500
C	5.65770500	-2.71663300	-1.09809400
H	3.61265600	-2.25926400	-0.63600600
C	6.98336900	-2.28720900	-1.05892600
H	5.40790100	-3.67414600	-1.54045500
H	7.77036900	-2.91204600	-1.46668800
N	-3.26944000	0.28697700	-0.74897700
C	-3.84356400	-0.83728000	-0.45763000
N	-3.19416000	-2.05652600	-0.36239400
C	-5.31673900	-0.81839000	-0.29872600
H	-2.18373200	-1.98348500	-0.31799000
H	-3.55435100	-2.67515200	0.34998000
C	-6.07186200	-1.99293300	-0.42443000
C	-5.98874500	0.38246600	-0.01996600
C	-7.45683800	-1.97039600	-0.26804900
C	-7.36916400	0.40175800	0.12962700
H	-5.40196400	1.28698100	0.07353100
C	-8.11262400	-0.77498100	0.01107500
H	-7.87028600	1.33930200	0.34768200
H	-9.19044100	-0.75693000	0.13462600
H	8.32263500	-0.71323800	-0.45342800
H	6.52787100	0.69850700	0.49064000
H	-5.57205600	-2.92129200	-0.67424600
H	-8.02300500	-2.89029700	-0.37348500
H	2.60904000	-1.34189800	1.06994300

U-M8-EtOH-cis

U	1.22274800	-0.11527400	-0.05925400
O	1.92795000	0.00224300	-1.69028200
O	0.33674900	-2.44555000	-0.59556500
O	2.29953400	-2.44196700	0.27938100
O	1.34342300	-4.34521500	-0.20243900
N	1.33489500	-3.13268400	-0.17064500
O	0.59934200	-0.21014600	1.60076600
O	2.82675100	1.76994400	0.70071400
O	3.67187000	-0.19945200	0.85815100
O	4.88858100	1.53585500	1.37800200
O	-0.81669200	0.08659400	-0.85426000
N	3.84631700	1.04567600	0.99605400
O	0.59871200	2.44177300	-0.26967400
H	1.43831600	2.89448900	-0.11342800
N	-2.05408000	0.45645800	-0.40330500
C	-2.90305200	-0.52025300	-0.34943100
N	-2.63763000	-1.81640700	-0.76339000
C	-4.27597700	-0.20292300	0.10663900
H	-1.65086500	-1.99031700	-0.92676200
H	-3.05674400	-2.53149200	-0.18531200
C	-5.35632300	-1.02979000	-0.23284200
C	-4.52540700	0.93543400	0.88967100
C	-6.64703200	-0.72997400	0.19918500
C	-5.81383300	1.23413600	1.31325900
H	-3.68858000	1.56866800	1.15418500
C	-6.88321900	0.40193100	0.97400300
H	-5.98626700	2.11670400	1.92070900
H	-7.88732500	0.63468300	1.31262200
H	-5.18314200	-1.89541000	-0.86118300
H	-7.46978300	-1.38100300	-0.07834200
C	-0.10633200	3.04218200	-1.36678000
C	-0.44374400	4.49744100	-1.07472500
H	-1.00664700	2.44340600	-1.48247500
H	0.49055800	2.95038300	-2.28205100
H	-1.02068300	4.92591900	-1.90058100
H	-1.03852800	4.57275100	-0.16139100
H	0.46009800	5.10335200	-0.94788400

U-M8-EtOH

U	-0.97450000	-0.04585300	-0.08445700
O	-1.71240400	0.17923100	-1.69207700
O	-2.46003400	-2.08796900	0.31887000

O	-0.57146600	-2.50561400	-0.62300200
O	-1.96482800	-4.14206300	-0.23379000
N	-1.67235600	-2.96579100	-0.18421000
O	-0.36854900	-0.22112600	1.57528800
O	-1.91174800	2.32248200	0.66446300
O	-0.00038000	2.38866100	-0.30678200
O	-0.95433300	4.25202400	0.31300600
O	1.04472900	-0.17406900	-0.86702100
N	-0.95117100	3.04132700	0.22432900
O	-3.53158700	0.34802800	0.75111100
H	-3.52365300	1.31326200	0.81074500
N	2.27665500	-0.58948600	-0.45284500
C	3.16895300	0.34843500	-0.47008000
N	2.94124300	1.64287500	-0.92255100
C	4.54195600	-0.01164900	-0.04944500
H	1.95272500	1.83679400	-1.04063600
H	3.39526200	2.35616700	-0.36828200
C	5.63822800	0.78397300	-0.41146400
C	4.77511100	-1.16163700	0.72212700
C	6.92897600	0.44571400	-0.00822800
C	6.06308600	-1.49793500	1.11695000
H	3.92658000	-1.77484900	0.99647500
C	7.14861200	-0.69467100	0.75859900
H	6.22317900	-2.38941000	1.71461200
H	8.15269100	-0.95797300	1.07437900
H	5.47796500	1.65485400	-1.03596500
H	7.76425000	1.07293700	-0.30291600
C	-4.67793000	-0.07803800	0.00029100
C	-5.97209500	0.22799300	0.74204100
H	-4.54594100	-1.14986500	-0.13374400
H	-4.66707400	0.39334500	-0.98932400
H	-6.83215300	-0.14977000	0.17957900
H	-5.96643300	-0.24510500	1.72685100
H	-6.10859100	1.30579300	0.87996400

U-M8-M8-cis

U	0.31297300	-1.30099800	0.05499900
O	-0.75332700	-1.40449600	1.48451200
N	2.31720100	1.35632300	0.59052800
O	-1.53709200	-2.54770900	-1.31753300
C	1.90723700	2.52957800	0.21546200
O	1.32720100	0.50517300	0.93120700
O	-0.21870400	-3.89692300	-0.27818200

N	-1.23739800	-3.75270000	-1.01010400
O	-1.90643900	-4.69872400	-1.40703800
O	1.31396200	-1.24466600	-1.41625900
N	-1.99266900	1.11007800	-0.32191400
O	1.94294200	-2.57089700	1.31158000
C	-3.23761300	0.80257000	-0.52094100
O	-1.10553100	0.25585300	-0.87706100
O	3.24589700	-3.57470800	-0.13762600
N	2.99564200	-3.28670300	1.03431700
O	3.69720200	-3.65484500	1.98366900
N	-3.65129800	-0.29278500	-1.29082400
H	-2.84925500	-0.87711800	-1.52075600
H	-4.35125700	-0.85405800	-0.81909700
C	-4.26742200	1.70452600	0.02249500
C	-5.60408800	1.61366500	-0.40215400
C	-3.94681500	2.68110300	0.98548500
C	-6.58293900	2.45907700	0.11857400
C	-4.92354200	3.52404600	1.49539800
H	-2.91819600	2.75284700	1.31478500
C	-6.25278400	3.41929700	1.07072700
H	-4.65018700	4.26665300	2.23919700
H	-7.01477800	4.07606400	1.47927700
N	0.56835800	2.93415700	0.21153100
H	0.29925900	3.39327900	-0.65070000
H	-0.05395400	2.14408400	0.36778900
C	2.93566000	3.52330200	-0.14278300
C	2.61731800	4.88713700	-0.25813500
C	4.26818000	3.13522200	-0.38124400
C	3.58900800	5.82535800	-0.60465400
C	5.23260100	4.07352000	-0.71887700
H	4.51083900	2.08406800	-0.29214400
C	4.90249700	5.42828700	-0.83851700
H	6.25278400	3.74748500	-0.89973400
H	5.65929500	6.15769600	-1.11114700
H	-7.60830700	2.36773900	-0.22897100
H	-5.86060400	0.88904400	-1.16573100
H	1.60410700	5.20703600	-0.04589900
H	3.31518600	6.87381100	-0.68472000

U-M8-M8

U	-0.03684500	0.40232100	-0.05470100
O	-0.77630000	0.21260200	-1.67000600
N	3.27119900	0.68127200	-0.64099200

O	-1.55094600	2.51837700	0.39534700
C	3.98005300	-0.40564100	-0.70704200
O	1.98639900	0.51906900	-1.03379200
O	0.31762700	2.96993300	-0.57806300
N	-0.77126500	3.40027200	-0.09818200
O	-1.06883400	4.58890600	-0.10491900
O	0.68967200	0.65073300	1.55548600
N	-3.11964300	-0.85092600	0.39106300
O	0.66050500	-1.96575900	-0.09056900
C	-4.16250200	-0.10163200	0.58023100
O	-1.97095400	-0.33272600	0.86803900
O	0.48498200	-2.80933800	1.92171500
N	1.02390400	-2.81985700	0.81830300
O	1.91089600	-3.63959800	0.51202300
N	-4.13148900	1.12058200	1.27179400
H	-3.15986100	1.36980200	1.44208700
H	-4.56378700	1.86847600	0.74007500
C	-5.46374400	-0.60362700	0.10899600
C	-6.66485400	-0.00750600	0.52989400
C	-5.54411200	-1.69145000	-0.78197800
C	-7.89705000	-0.47498300	0.07465700
C	-6.77296100	-2.15628400	-1.22696000
H	-4.61738200	-2.14830100	-1.10488600
C	-7.96261400	-1.55046500	-0.80673300
H	-6.80774000	-2.99555600	-1.91558200
H	-8.92158900	-1.91317600	-1.16431800
N	3.50358800	-1.62251700	-1.20282100
H	3.64156800	-2.40129200	-0.56515800
H	2.49959100	-1.54799400	-1.35172100
C	5.40036000	-0.31232300	-0.32015800
C	6.29944400	-1.34734200	-0.62616000
C	5.89689100	0.81229500	0.36593500
C	7.64172600	-1.26395500	-0.25889000
C	7.23514900	0.89361400	0.72330000
H	5.20064100	1.60660700	0.60288300
C	8.12114000	-0.14535600	0.41749400
H	7.59346900	1.77096300	1.25436500
H	9.16579700	-0.08157300	0.70733500
H	-8.81040700	0.00309400	0.41800600
H	-6.62014700	0.81057300	1.23887200
H	5.93383300	-2.20752700	-1.17369200
H	8.31580700	-2.07906400	-0.50756000

U-M9-M9-T2

U	0.08239700	-0.90882400	0.08512700
O	-0.00169500	-0.93865400	1.87089800
O	-0.08602500	-1.06159700	-1.68582400
O	-1.83823300	-2.56282800	0.20445200
H	-2.16206600	-2.82371700	1.07385600
C	-2.60951300	-3.21039000	-0.84300200
C	-4.07957200	-2.84238600	-0.76572200
H	-2.45664400	-4.29095300	-0.76581200
H	-2.15338100	-2.86161800	-1.76813300
H	-4.62398700	-3.31597200	-1.58736600
H	-4.52897600	-3.18775100	0.17100700
H	-4.21481400	-1.76162600	-0.83864900
O	1.98435000	-2.17616800	0.10926400
N	2.47560100	-0.89873700	0.03548900
C	3.76121300	-0.75616000	0.03613800
N	4.58472200	-1.85895000	0.01935400
C	4.35164200	0.59657000	-0.01006900
H	5.46088900	-1.76967700	0.51069200
H	4.07793200	-2.71867500	0.19066500
C	5.66167100	0.77855400	-0.47475600
C	3.61577400	1.71617400	0.40663200
C	6.22911600	2.04930500	-0.51175000
H	6.22618000	-0.07196200	-0.83832100
C	4.18674100	2.98198000	0.36174400
H	2.60060800	1.58954300	0.76034900
C	5.49492300	3.15493800	-0.09173000
H	7.24164900	2.17466300	-0.87872200
H	3.60870200	3.83922000	0.68826500
H	5.93617700	4.14493900	-0.12019200
N	-1.20394000	1.15949100	0.08381500
C	-1.97323800	2.18562600	-0.08732300
O	0.14409700	1.37955700	0.00239900
N	-1.45141700	3.41171700	-0.43293300
C	-3.43693000	2.03096000	0.02667700
H	-1.91899600	4.22230100	-0.05630700
H	-0.44035100	3.42776700	-0.37825300
C	-4.29754600	2.83507000	-0.73325800
C	-3.98801300	1.08813300	0.90617900
C	-5.67789400	2.69266600	-0.62145800
H	-3.87920800	3.55212200	-1.42965900
C	-5.36726500	0.94679200	1.01107400
H	-3.32284200	0.48937200	1.51586400
C	-6.21759800	1.74849000	0.24893000

H	-6.33214300	3.31575500	-1.22082400
H	-5.78233500	0.22160000	1.70234200
H	-7.29271900	1.64138300	0.33810900

U-M9-M9-T3

U	-0.01670400	-0.93526600	-0.10681700
O	-0.03301700	-1.00977300	1.67721300
O	-0.00451000	-0.58087200	-1.85727500
O	-0.07324100	1.54223400	0.38599900
H	-0.20244800	1.71806300	1.32515000
C	-0.27632000	2.74561800	-0.39167900
C	0.64159100	3.86574100	0.06405300
H	-1.32911100	3.03448000	-0.32162800
H	-0.06989000	2.44765500	-1.41926000
H	0.49850600	4.74631400	-0.56848700
H	0.42465800	4.16141000	1.09534900
H	1.68785800	3.55974800	0.00573600
O	-1.88567400	-2.23015500	-0.24455500
N	-2.46560600	-0.99287800	-0.15565700
C	-3.74395400	-0.96776500	0.04020600
N	-4.45709500	-2.12579000	0.24870100
C	-4.44515400	0.33060000	0.09829300
H	-5.39853000	-2.14687900	-0.11275100
H	-3.90518500	-2.95688000	0.07495700
C	-5.54610100	0.50796200	0.94691400
C	-4.02835900	1.39886600	-0.70820000
C	-6.20725400	1.73227400	0.99644200
H	-5.86434000	-0.30936500	1.58333600
C	-4.69146700	2.62031100	-0.65418600
H	-3.19924800	1.24744400	-1.38821300
C	-5.78239600	2.79207500	0.19828100
H	-7.05235300	1.85950800	1.66360500
H	-4.36998400	3.43546300	-1.29332400
H	-6.30189800	3.74296000	0.23360700
N	2.43020800	-1.02353200	-0.13458600
C	3.71000200	-1.01624000	0.05307000
O	1.83405900	-2.25448800	-0.22138800
N	4.40684200	-2.18475400	0.25763200
C	4.43325600	0.27032200	0.10144600
H	5.34648400	-2.21896100	-0.10729100
H	3.84229500	-3.00775000	0.08632800
C	4.02201800	1.34664300	-0.69679200
C	5.55225900	0.42642400	0.93047200

C	4.71036800	2.55446200	-0.65569700
H	3.17571400	1.21315800	-1.35911200
C	6.23806100	1.63745000	0.96776900
H	5.86564600	-0.39646500	1.56213000
C	5.82004400	2.70488000	0.17638200
H	4.39239300	3.37603400	-1.28821000
H	7.09687000	1.74836900	1.62017800
H	6.35837800	3.64556000	0.20189100

U-M9-M9-T1

U	1.47830700	-0.46367500	-0.11346000
O	1.48385000	-0.57870800	-1.89365500
O	1.65366400	-0.37526800	1.66011200
O	3.99510000	-0.54237700	-0.24946700
H	4.34530300	-0.37785000	-1.13287800
C	4.93035900	-0.06186700	0.75654200
C	5.19292500	1.42652700	0.61604200
H	5.84782900	-0.65230600	0.67586800
H	4.44836900	-0.29455100	1.70482700
H	5.86396500	1.75981600	1.41286800
H	5.67248500	1.65742800	-0.34072500
H	4.25752800	1.98522200	0.68171400
O	0.85708600	-2.64986400	0.05056200
N	-0.37503800	-2.04918000	-0.02321300
C	-1.39829600	-2.83583300	0.06996600
N	-1.23540900	-4.17408100	0.34662000
C	-2.76605100	-2.29839400	-0.07500900
H	-1.90735300	-4.80198500	-0.06729600
H	-0.26828200	-4.46733600	0.28579700
C	-3.83534800	-2.89346400	0.60967500
C	-3.01949900	-1.20800200	-0.91786900
C	-5.12968700	-2.40594000	0.45438300
H	-3.64405700	-3.72247000	1.28096900
C	-4.31362500	-0.72253400	-1.06660500
H	-2.19869200	-0.75722000	-1.46106000
C	-5.37295900	-1.32044700	-0.38465600
H	-5.94725600	-2.87092200	0.99394800
H	-4.49591000	0.12224800	-1.72043600
H	-6.38188600	-0.94302100	-0.50791900
N	0.49985700	1.76251000	-0.09382500
C	-0.12039200	2.89736700	-0.13357000
O	1.85937800	1.80343700	-0.27344100
N	0.55003300	4.05427800	-0.46251300

C	-1.57163100	2.96516800	0.12978500
H	0.23047100	4.89925800	-0.01407400
H	1.55367800	3.92512200	-0.48557500
C	-2.35622500	3.95037000	-0.48687300
C	-2.17866900	2.06947400	1.02030100
C	-3.71906200	4.03581700	-0.21776800
H	-1.89821400	4.63189900	-1.19417200
C	-3.54117600	2.15620100	1.28200300
H	-1.57273600	1.31920500	1.51211800
C	-4.31516100	3.14037700	0.66793600
H	-4.31619600	4.79847000	-0.70512600
H	-3.99876900	1.45651200	1.97152700
H	-5.37623400	3.20917900	0.87986700

U-M9-M10-T1

U	1.21180100	-0.75671700	0.01311400
O	0.85409100	-0.90444300	-1.72951700
O	1.61232200	-0.65602100	1.75105600
O	3.42496900	-1.90094000	-0.39204500
H	3.68041700	-2.00405400	-1.31594500
C	4.60943500	-1.82557900	0.44869800
C	5.46941700	-0.62375000	0.10189800
H	5.15655400	-2.76765800	0.35014400
H	4.21781100	-1.75749500	1.46254500
H	6.32455200	-0.57201800	0.78192600
H	5.85990500	-0.69465800	-0.91837200
H	4.88975600	0.29695700	0.19096600
O	2.47141900	1.14173400	-0.42589200
N	1.24529900	1.65712500	-0.11882600
C	1.05419600	2.91439900	-0.35794500
N	2.01379700	3.67190400	-0.98718500
C	-0.24077900	3.53349600	-0.00963400
H	2.07696000	4.64130300	-0.71621700
H	2.89583700	3.18436400	-1.08127400
C	-0.79936800	4.52132000	-0.83222200
C	-0.92281300	3.15063700	1.15443000
C	-2.02298500	5.09937000	-0.50605700
H	-0.28226100	4.81397600	-1.73846900
C	-2.14697000	3.72963600	1.47458000
H	-0.46762500	2.42052900	1.81291300
C	-2.70185500	4.70422400	0.64480500
H	-2.44983200	5.85506000	-1.15569700
H	-2.66013900	3.43469400	2.38311500

H	-3.65275100	5.15827200	0.89903800
N	-1.38406000	-2.70411200	0.21860700
C	-2.07389500	-1.61957300	0.14299200
O	-0.07370600	-2.54364500	0.41278900
N	-1.38430000	-0.33592400	0.25795100
C	-3.53448000	-1.67309700	-0.03842100
H	-1.66234400	0.28751500	-0.49721700
C	-4.18469500	-2.91132600	-0.19878300
C	-4.31446300	-0.50739800	-0.05274700
C	-5.55964900	-2.97105400	-0.36579100
H	-3.58794000	-3.81378500	-0.18871300
C	-5.69686200	-0.57360500	-0.22135200
H	-3.85210400	0.46512100	0.07078200
C	-6.32630300	-1.80289300	-0.37865900
H	-6.04064800	-3.93522100	-0.48855100
H	-6.27836500	0.34162300	-0.22936800
H	-7.40095700	-1.85491900	-0.51107100
H	-1.64801400	0.13308600	1.12327100

U-M9-M10-T2

U	-0.13097000	0.67386400	-0.22314900
O	-0.24172600	0.86726100	-1.99694900
O	0.18638800	0.68517700	1.53599800
O	0.54068100	3.13513000	-0.23724300
H	0.21898700	3.57094300	-1.03554600
C	0.45195600	4.05058500	0.89046200
C	-0.93425100	4.65225300	1.03031500
H	1.21994900	4.82003600	0.76261100
H	0.70853300	3.44054500	1.75554100
H	-0.96377300	5.30754100	1.90552800
H	-1.19433000	5.25709200	0.15524800
H	-1.68100900	3.86538800	1.14656100
O	-2.18230200	1.71634700	0.08748700
N	-2.48423500	0.38108000	0.06898200
C	-3.73037800	0.04414200	0.16270700
N	-4.71225600	1.00582800	0.18644300
C	-4.11019400	-1.38248700	0.17575700
H	-5.53713700	0.79593600	0.72692100
H	-4.34074400	1.94052400	0.29650700
C	-5.37454800	-1.77872600	-0.28213200
C	-3.21890400	-2.35923400	0.64209900
C	-5.73961900	-3.12177500	-0.27178200
H	-6.05884300	-1.03656400	-0.67626500
C	-3.58564400	-3.69948300	0.64254300

H	-2.24429900	-2.06373900	1.00907700
C	-4.84716800	-4.08595600	0.18998400
H	-6.71792600	-3.41483500	-0.63571900
H	-2.88538100	-4.44403300	1.00319200
H	-5.13063500	-5.13231100	0.19590300
N	2.01292700	-1.79837800	-0.18527200
C	2.92704200	-0.89266200	-0.22786600
O	0.76978800	-1.36119300	-0.39850500
N	2.53711500	0.48688700	-0.50744700
C	4.33971700	-1.24497100	-0.00757900
H	3.05422300	1.12793900	0.08891600
C	4.68684400	-2.53315800	0.44086700
C	5.37092500	-0.32275000	-0.23877600
C	6.01455500	-2.87593700	0.64580600
H	3.89530000	-3.24823900	0.62184000
C	6.70411800	-0.67195600	-0.02955900
H	5.14490100	0.67508800	-0.59743900
C	7.03290500	-1.94789900	0.41364800
H	6.26048900	-3.87339400	0.99295900
H	7.48402200	0.05749700	-0.21774200
H	8.06918700	-2.22005300	0.57812700
H	2.76612600	0.72956000	-1.47073100

U-M9-M10-T2'

U	-0.02676000	0.48101600	0.14487400
O	0.05315400	0.50081500	1.93014200
O	0.02060300	0.58440800	-1.63753100
O	1.54598700	2.46853500	0.19737800
H	1.72323900	2.87936100	1.05102800
C	1.97349400	3.34221800	-0.88291300
C	3.46942800	3.59225700	-0.83632400
H	1.40202000	4.27284400	-0.82338200
H	1.67851200	2.81668700	-1.78975800
H	3.76744400	4.21851100	-1.68173600
H	3.75897700	4.11525000	0.08074900
H	4.02172100	2.65207300	-0.89048100
O	0.38414000	-1.78124400	0.07217500
N	1.65322100	-1.27602700	0.10480200
C	2.62690500	-2.10957700	-0.06696700
N	2.38464500	-3.43163500	-0.36491100
C	4.02176100	-1.62925400	-0.00390300
H	3.04058200	-4.10248900	0.00559000
H	1.40829800	-3.67839400	-0.26299500
C	5.01689100	-2.23734600	-0.78129300

C	4.37358600	-0.56809900	0.84201000
C	6.33297600	-1.78788800	-0.71941700
H	4.74983400	-3.04489600	-1.45272500
C	5.68882900	-0.12040000	0.89738400
H	3.61106800	-0.11777800	1.46508100
C	6.67356900	-0.72847800	0.11828100
H	7.09144800	-2.26211000	-1.33198100
H	5.95116000	0.69453600	1.56291900
H	7.69946400	-0.38176200	0.16875500
N	-3.18309200	1.37726000	0.08999700
C	-3.42566000	0.11277100	0.03950200
O	-1.89545800	1.71037000	0.18866500
N	-2.29998500	-0.81115400	0.09046400
C	-4.80803900	-0.38219600	-0.06287200
H	-2.35064800	-1.41625300	0.90827400
C	-5.88534300	0.52164200	-0.12841700
C	-5.09123900	-1.75548800	-0.09622800
C	-7.18938000	0.06073400	-0.22279100
H	-5.67276400	1.58224600	-0.10323000
C	-6.40448500	-2.21340300	-0.19112200
H	-4.28780400	-2.48134700	-0.04712300
C	-7.45912200	-1.31001100	-0.25479300
H	-8.00497900	0.77379600	-0.27221700
H	-6.59819800	-3.28004600	-0.21488600
H	-8.48062100	-1.66520300	-0.32883700
H	-2.28279800	-1.42555200	-0.72135300

U-M10-M10-T1

U	0.02425300	0.91143100	-0.29495100
O	0.47118200	0.87857200	1.43446700
O	-0.42862300	0.69694200	-2.00670900
O	-0.44221600	3.40199000	-0.22450700
H	-1.38314100	3.39903300	0.01501300
C	0.26781400	4.49327700	0.40633100
C	0.09436000	4.49816200	1.91541800
H	-0.07892500	5.42859700	-0.04346900
H	1.31092000	4.34783200	0.12424700
H	0.67186200	5.31719200	2.35345600
H	-0.95445200	4.64221600	2.19221600
H	0.43929500	3.55695800	2.34760700
O	2.15802300	1.30835300	-0.81902200
N	3.24242200	0.58419200	-0.50394800
C	3.02974000	-0.67821800	-0.38041300

N	1.68108300	-1.19227400	-0.61046600
C	4.12589800	-1.59212800	-0.01803900
H	1.53779600	-2.03997100	-0.06967900
C	4.01655600	-2.97966000	-0.19171300
C	5.32400600	-1.07748500	0.50933100
C	5.06770500	-3.82785500	0.15127400
H	3.11861400	-3.41198200	-0.61945400
C	6.36871300	-1.92543900	0.84538600
H	5.41171700	-0.00786800	0.64689200
C	6.24687500	-3.30603600	0.67166600
H	4.96279600	-4.89693900	0.00456600
H	7.28372000	-1.50991400	1.25242900
H	7.06405600	-3.96525500	0.94088100
N	-3.23075700	0.65772600	0.23194800
C	-3.01733200	-0.61032000	0.22916200
O	-2.14846500	1.43747900	0.22089400
N	-1.63773400	-1.10359700	0.22955600
C	-4.14388300	-1.55935600	0.23299900
H	-1.40635000	-1.47199000	1.15203100
C	-5.45947900	-1.09569800	0.04535500
C	-3.94671300	-2.93488700	0.42437400
C	-6.52779800	-1.97929600	0.05199400
H	-5.61821800	-0.03615100	-0.10508400
C	-5.02419800	-3.81937900	0.42821800
H	-2.95058300	-3.33120400	0.58610300
C	-6.31835500	-3.34751300	0.24194200
H	-7.53324500	-1.60145300	-0.09652400
H	-4.84655100	-4.87811200	0.58025000
H	-7.15664300	-4.03459100	0.24274800
H	1.56707400	-1.43698700	-1.59434300
H	-1.55878000	-1.87903000	-0.42473300

U-M10-M10-T3

U	-0.00821600	-0.27671600	0.01336700
O	0.34320900	-0.33701700	1.77070400
O	-0.35747400	0.19725900	-1.67967200
O	0.02569600	2.26878300	0.45532900
H	0.17205900	2.54388300	1.36724800
C	-0.40485300	3.38961400	-0.35497700
C	0.63589700	4.49419500	-0.39559100
H	-1.35947200	3.76292000	0.03121400
H	-0.57818200	2.96172300	-1.34150600
H	0.28621900	5.31248200	-1.03064200
H	0.82357600	4.90562600	0.60098900

H	1.58036000	4.12748700	-0.80334700
O	-1.59848700	-1.83346500	0.03957000
N	-2.92659300	-1.74237800	-0.08647800
C	-3.42876600	-0.60113400	0.23123400
N	-2.53264800	0.44396600	0.71239700
C	-4.87558500	-0.35787700	0.11474800
H	-2.87046800	1.35801200	0.42641900
C	-5.48416200	0.76098300	0.70267700
C	-5.68681200	-1.26108400	-0.59668900
C	-6.85633800	0.97461200	0.58352500
H	-4.89596600	1.46705100	1.27873800
C	-7.05204800	-1.04582200	-0.70922500
H	-5.22145700	-2.12488500	-1.05282500
C	-7.64624200	0.07438800	-0.12273200
H	-7.30550400	1.84445900	1.04981200
H	-7.65956100	-1.75289000	-1.26301800
H	-8.71322400	0.24023600	-0.21745500
N	2.89365600	-1.73029400	-0.33093200
C	3.40458700	-0.55068600	-0.27381300
O	1.56555700	-1.76758800	-0.48357900
N	2.51589000	0.59786800	-0.40401500
C	4.85302900	-0.36770800	-0.08714200
H	2.83449800	1.36621300	0.17886800
C	5.65927500	-1.45985900	0.28345300
C	5.46786500	0.87900900	-0.27415900
C	7.02604200	-1.30178300	0.45554000
H	5.18889900	-2.42314700	0.43035700
C	6.84175400	1.03328100	-0.09687500
H	4.88241800	1.73912600	-0.57969700
C	7.62685300	-0.05429300	0.26904400
H	7.62979400	-2.15553900	0.74246000
H	7.29575300	2.00593200	-0.25067500
H	8.69514100	0.06475300	0.40883500
H	2.51220300	0.93281800	-1.36705300
H	-2.50434300	0.43865800	1.73177100

U-M10-M10-T2

U	0.00661900	0.38800100	0.32209600
O	-0.08724200	-0.30169800	-1.31557900
O	0.04639000	1.12188400	1.94732400
O	-0.24078800	2.80245200	-0.60356900
H	0.70468000	2.79434800	-0.85462900
C	-0.50009500	3.98188100	0.19235600

C	-0.28801000	5.25095800	-0.61493000	O	-0.03068100	0.77398200	1.77322200
H	0.13365600	3.96099300	1.08360000	O	-0.09842900	0.81329300	-1.78775200
H	-1.53862000	3.89362200	0.51626000	O	2.04845100	2.19051300	0.02902800
H	-0.53341100	6.12793200	-0.00920000	H	1.63339400	3.03420400	0.26188100
H	0.75478200	5.34438900	-0.93096500	O	-0.30681800	3.46881300	0.00094300
H	-0.92012400	5.25572700	-1.50572200	H	-1.10055900	3.38447400	0.55005100
O	1.95872500	1.48173300	-0.28975900	C	-0.69958900	4.08089000	-1.25673400
N	3.14980100	0.91561500	-0.53141000	C	-1.04666100	5.54849700	-1.07423900
C	3.32791200	-0.26363700	-0.05041500	H	-1.53449300	3.51146900	-1.66934600
N	2.25139700	-0.89962300	0.71135100	H	0.15909300	3.95163000	-1.91593200
C	4.60641800	-0.96825600	-0.25276700	H	-1.29746900	5.99664600	-2.04002000
H	2.14988400	-1.87347200	0.43061200	H	-1.91163800	5.67119700	-0.41562100
C	4.89475800	-2.16990800	0.41054500	H	-0.20691600	6.10104200	-0.64576200
C	5.57691500	-0.43747000	-1.12258700	C	3.34915900	2.08214700	0.63914800
C	6.11155600	-2.82088100	0.21423000	C	3.29188500	2.21033600	2.15313200
H	4.17799700	-2.60812500	1.09560100	H	4.00253700	2.84425000	0.20011400
C	6.78606200	-1.08852700	-1.31340800	H	3.72577600	1.10616300	0.33728600
H	5.35873600	0.48775700	-1.63909200	H	4.29002400	2.07540200	2.58036600
C	7.06183500	-2.28519800	-0.64733600	H	2.93351900	3.20024900	2.45296800
H	6.31244300	-3.74779400	0.73949200	H	2.61944900	1.46368000	2.57971500
H	7.51981100	-0.66399700	-1.98953400	O	-2.24846500	1.66827700	0.08600700
H	8.00723300	-2.79230600	-0.80214900	N	-2.50510400	0.32561200	0.09561800
N	-2.38839000	-1.75893900	0.74422300	C	-3.74168400	-0.04469200	0.16549300
C	-3.16356300	-0.86450300	0.23972600	N	-4.75468200	0.89253700	0.14848500
O	-1.17336800	-1.32660100	1.10250000	C	-4.08667200	-1.48012700	0.20242000
N	-2.66633000	0.50424400	0.09309500	H	-5.56811200	0.67057000	0.70259500
C	-4.53527200	-1.21131200	-0.17174900	H	-4.40052300	1.83284000	0.27037900
H	-2.90700500	0.86502200	-0.82781900	C	-5.36440600	-1.90638400	-0.18683700
C	-4.96815100	-2.54988300	-0.13513800	C	-3.15046200	-2.43500600	0.62711600
C	-5.44136600	-0.23148300	-0.60236100	C	-5.70543000	-3.25543000	-0.14132800
C	-6.25835900	-2.88531000	-0.51583400	H	-6.08263500	-1.18360800	-0.55580800
H	-4.27315600	-3.31031700	0.19534400	C	-3.49734800	-3.78013000	0.66582700
C	-6.73734800	-0.57413900	-0.98431200	H	-2.15557800	-2.12056900	0.91516300
H	-5.14872200	0.81159900	-0.63857000	C	-4.77432000	-4.19699500	0.28812200
C	-7.15196200	-1.90030500	-0.94373000	H	-6.69600700	-3.56958400	-0.45081200
H	-6.57186300	-3.92272300	-0.48210900	H	-2.76661400	-4.50852100	0.99978500
H	-7.42050100	0.20087000	-1.31313900	H	-5.03897200	-5.24786400	0.32529300
H	-8.15887500	-2.16778400	-1.24280400	N	1.30787700	-1.31971300	-0.01100600
H	2.47939000	-0.90839500	1.70554900	C	2.05978300	-2.31031300	-0.37707300
H	-3.11832900	1.11316600	0.77451100	O	-0.04269900	-1.56058800	-0.07231500
				N	1.51659500	-3.46435800	-0.88673200
				C	3.53042400	-2.20074500	-0.29042700
				H	2.00138800	-4.32658100	-0.69304900
				H	0.50728000	-3.48978800	-0.81277900
Cis-U-M9-M9-T2							
U	-0.11974500	0.71084600	-0.01008800				

C	4.34310000	-2.75991000	-1.28628800
C	4.13338500	-1.56759900	0.80429400
C	5.72900500	-2.67076500	-1.19595200
H	3.88102400	-3.24250100	-2.13951800
C	5.51977700	-1.48166900	0.89068900
H	3.50397600	-1.16830500	1.59008200
C	6.32177400	-2.03110300	-0.10883100
H	6.34682100	-3.09668500	-1.97853500
H	5.97614300	-0.99923600	1.74800800
H	7.40165900	-1.96731400	-0.03725200

Cis-U-M9-M9-T3

U	0.02178000	-0.48283200	-0.11590000
O	-0.13544900	-0.60550800	1.66043900
O	0.12168300	-0.11349300	-1.86152800
O	1.12031800	1.83901200	0.58945400
H	0.31231100	2.32516400	0.80259400
O	-1.48537200	1.79367700	-0.10782100
H	-2.37604300	1.50082300	0.12890000
C	-1.55532500	2.60092200	-1.31103400
C	-2.28438200	3.91109500	-1.06456300
H	-2.02223300	2.01747900	-2.10815800
H	-0.51720300	2.76834300	-1.59594800
H	-2.29580300	4.50986600	-1.97989500
H	-3.32101100	3.73852900	-0.76220000
H	-1.79190900	4.49309400	-0.28171900
C	2.09820600	2.05890200	1.63404000
C	1.48395500	2.01717200	3.02311000
H	2.58977900	3.01935000	1.44455600
H	2.83777900	1.27116800	1.50423500
H	2.26235400	2.16390600	3.77742500
H	0.74476800	2.81555300	3.15374700
H	0.99611900	1.05775100	3.19995100
O	-1.41153100	-2.24427100	-0.40923900
N	-2.32368100	-1.23456300	-0.32113400
C	-3.53533700	-1.59077700	-0.02795200
N	-3.84311300	-2.89978500	0.26199000
C	-4.59239600	-0.56531800	0.07151600
H	-4.74668400	-3.23229900	-0.03888800
H	-3.06437900	-3.52272100	0.08104100
C	-5.57027700	-0.64638600	1.07343500
C	-4.64551200	0.49698700	-0.84333400
C	-6.56195400	0.32500200	1.17037300

H	-5.53225100	-1.46297700	1.78457200
C	-5.64015000	1.46700600	-0.74144900
H	-3.92859100	0.52300500	-1.65533900
C	-6.59921100	1.38643700	0.26729600
H	-7.30513700	0.25630500	1.95679200
H	-5.68172800	2.27303000	-1.46584400
H	-7.37649800	2.13830700	0.34143900
N	2.38844100	-1.12291900	-0.15885400
C	3.65021900	-1.41089800	-0.16552600
O	1.52934500	-2.18412600	-0.21252800
N	4.07486600	-2.72093600	-0.08754400
C	4.65955700	-0.33411100	-0.20350800
H	4.91299200	-2.94567700	-0.60258800
H	3.30847700	-3.37295600	-0.20908700
C	4.40436400	0.85912900	-0.89474300
C	5.89892500	-0.50038500	0.43114200
C	5.36386200	1.86491700	-0.93594800
H	3.45645600	0.97968600	-1.40406000
C	6.85667400	0.50867500	0.38414100
H	6.09678300	-1.41409100	0.97928200
C	6.59278800	1.69440600	-0.29827600
H	5.15729800	2.78021100	-1.47951800
H	7.80792800	0.37014100	0.88583700
H	7.34104800	2.47801600	-0.33808300

Cis-U-M9-M9-T1

U	1.29944000	-0.04156200	-0.02204900
O	1.33827500	0.05062200	1.75987600
O	1.38492300	-0.10048600	-1.80150300
O	3.59590200	-1.25160700	0.15149400
H	4.13924200	-0.69773400	0.72529200
O	3.49407700	1.46477100	0.06927000
H	2.95642800	2.21558500	0.36899900
C	4.15366800	1.83672600	-1.16572100
C	5.23327900	2.87925800	-0.92673300
H	3.40363400	2.18900800	-1.87844300
H	4.57641100	0.90882900	-1.55188400
H	5.74961200	3.10732900	-1.86371300
H	4.80549500	3.81139500	-0.54598800
H	5.97044100	2.51983000	-0.20475900
C	3.86340000	-2.65030300	0.40252500
C	3.63530200	-3.03090500	1.85504500
H	4.88924500	-2.86440800	0.08325600

H	3.17535800	-3.18238100	-0.25161900	O	1.83509800	-1.84552400	0.03346500
H	3.84264800	-4.09591600	1.99720300	H	-0.82946100	2.69434700	-0.11554400
H	4.29766500	-2.47163700	2.52411300	H	2.73365200	-1.49317600	0.06204600
H	2.60046100	-2.83390700	2.13716700	C	1.75676600	-3.05771600	0.82067500
O	1.00249100	2.27797300	-0.13123800	C	2.17906100	-2.83043600	2.26263000
N	-0.27755600	1.84292000	0.08297800	H	2.37410200	-3.82084200	0.33480600
C	-1.18913200	2.75520000	0.17817900	H	0.71321500	-3.35961000	0.75492600
N	-0.89036400	4.07996600	-0.06614300	H	2.07235100	-3.75796300	2.83302700
C	-2.57922400	2.39421600	0.51998600	H	3.22652000	-2.51826800	2.32739300
H	-1.39444200	4.75593600	0.48781700	H	1.55651200	-2.06190100	2.72401800
H	0.10680700	4.23865300	-0.13508300	C	-2.22727300	2.39635000	1.26241000
C	-3.64764200	3.17448100	0.05572100	C	-2.90191400	3.75247200	1.14761400
C	-2.84710100	1.29462300	1.34654500	H	-1.52131200	2.36513400	2.09695000
C	-4.95611000	2.86070500	0.41228900	H	-2.96006100	1.60339400	1.40727300
H	-3.45015700	4.01350200	-0.60136200	H	-3.44937400	3.97753000	2.06739500
C	-4.15577800	0.98379000	1.69615800	H	-2.16761000	4.54949900	0.99367500
H	-2.02299700	0.69876800	1.71745100	H	-3.60756600	3.76529900	0.31430100
C	-5.21367600	1.76599400	1.23458100	O	1.13694000	2.07935400	-0.03445900
H	-5.77434200	3.46888500	0.04275700	N	2.17271400	1.21426900	-0.17806300
H	-4.35021100	0.12913900	2.33351900	C	3.36987100	1.69425000	-0.09180000
H	-6.23260000	1.52263800	1.51382700	N	3.59281300	3.01518600	0.24171900
N	-0.36462200	-1.81527400	-0.11759700	C	4.52356100	0.79254700	-0.28245000
C	-1.32265000	-2.67922700	-0.21126600	H	4.37845300	3.45845700	-0.21138700
O	0.89220500	-2.31443800	0.08903400	H	2.73653900	3.55563500	0.22827700
N	-1.08797900	-4.01710700	0.03132900	C	5.69925400	0.97166700	0.45989500
C	-2.69391100	-2.24854300	-0.54736000	C	4.46313800	-0.25122000	-1.21981500
H	-1.62875200	-4.66613400	-0.52035900	C	6.78126100	0.11402900	0.28273100
H	-0.09846000	-4.22334300	0.08940800	H	5.74931200	1.77086100	1.18996000
C	-3.79801600	-2.97617900	-0.08069000	C	5.54618100	-1.11027700	-1.38648900
C	-2.91107500	-1.13443400	-1.36953100	H	3.57682500	-0.35900300	-1.83406400
C	-5.09089300	-2.59710900	-0.43051500	C	6.70790200	-0.93148600	-0.63598500
H	-3.63952300	-3.82595200	0.57315800	H	7.68138300	0.25796800	0.86979400
C	-4.20425900	-0.75831300	-1.71250600	H	5.48882600	-1.90819900	-2.11833200
H	-2.06064900	-0.57828700	-1.74265500	H	7.55276000	-1.59668000	-0.77290100
C	-5.29772100	-1.48862600	-1.24856100	O	-1.04974500	-2.05868400	-0.10368700
H	-5.93653200	-3.16525400	-0.05894500	N	-2.10065500	-1.19167800	-0.13527700
H	-4.35888300	0.10699500	-2.34641600	C	-3.28536600	-1.70769500	-0.17745100
H	-6.30452900	-1.19420600	-1.52256700	N	-3.46334600	-3.07407000	-0.07679400
				C	-4.47497700	-0.83905500	-0.27926700
				H	-4.22611000	-3.45477200	-0.61732900
				H	-2.58717100	-3.57299400	-0.17382000
				C	-5.70023300	-1.25355600	0.26251700
				C	-4.40658400	0.39820300	-0.93652500
				C	-6.83065300	-0.44855900	0.15223300
Trans-U-M9-M9-T2							
U	0.03459800	-0.01221400	-0.08633100				
O	0.02551500	0.04079200	-1.86624100				
O	-1.53332400	2.04740500	0.04081000				
O	0.03266400	-0.01659800	1.69959400				

H	-5.75661500	-2.19756700	0.79169200
C	-5.53860800	1.19926400	-1.04021000
H	-3.46651200	0.71931500	-1.36615700
C	-6.75457100	0.77991900	-0.49970100
H	-7.76957900	-0.77942400	0.58194300
H	-5.47503500	2.14943300	-1.55895900
H	-7.63583000	1.40507300	-0.58953900

Trans-U-M9-M9-T1

U	0.00700100	-1.01202900	-0.16687800
O	0.04114300	-0.77449100	-1.93040400
O	0.21781100	1.54808200	0.17634600
O	-0.00381300	-1.11966700	1.61757500
O	0.08787900	-3.57109200	-0.28313000
H	1.14165500	1.79048000	0.02867300
H	1.02233100	-3.76440900	-0.13166400
C	-0.75279200	-4.53608000	0.38123100
C	-0.40804400	-4.68345400	1.85441300
H	-0.66631100	-5.49126200	-0.14844900
H	-1.76441900	-4.15622700	0.24875900
H	-1.08994200	-5.39465700	2.33002500
H	0.61160900	-5.05996700	1.98825800
H	-0.49059500	-3.72171000	2.36358100
C	-0.25497400	2.19782400	1.38178400
C	-0.16118900	3.70957000	1.27402300
H	0.30706100	1.81572100	2.23932300
H	-1.28855800	1.87238000	1.48735600
H	-0.55054200	4.17218900	2.18551600
H	0.87539800	4.03616600	1.14764000
H	-0.74718000	4.07291500	0.42800100
O	2.15063100	-1.94368600	-0.28458700
N	2.46597500	-0.63755500	-0.07739500
C	3.68863800	-0.28673200	-0.31700700
N	4.60031800	-1.17124400	-0.85111800
C	4.10013800	1.11059100	-0.07653600
H	5.55294300	-1.08570900	-0.52989500
H	4.23933000	-2.11643000	-0.88630400
C	5.00672200	1.74542400	-0.93728500
C	3.60252200	1.81811700	1.02835000
C	5.38961500	3.06372100	-0.70856800
H	5.38862600	1.20575800	-1.79573800
C	3.98785600	3.13768500	1.25103600
H	2.94746500	1.30806900	1.72480300

C	4.88019900	3.76552000	0.38265700
H	6.08276800	3.54668100	-1.38808900
H	3.60871400	3.66952200	2.11666000
H	5.18385500	4.79066400	0.56108500
O	-2.15646400	-1.81671100	-0.23148100
N	-2.39030000	-0.47504600	-0.20144400
C	-3.62623800	-0.09627500	-0.19820100
N	-4.65183400	-1.01718500	-0.09983400
C	-3.96183900	1.34034200	-0.25349600
H	-5.48900500	-0.79365800	-0.61785900
H	-4.31710100	-1.96434700	-0.22956800
C	-5.12094200	1.82392600	0.37002400
C	-3.14310500	2.23601600	-0.95645200
C	-5.44980000	3.17479600	0.29817300
H	-5.74930800	1.14000500	0.92848300
C	-3.47702000	3.58445200	-1.02462200
H	-2.25760000	1.86076300	-1.45376200
C	-4.63026000	4.05946400	-0.39925400
H	-6.34507300	3.53664200	0.79143500
H	-2.84342700	4.26512900	-1.58255500
H	-4.89032300	5.11022500	-0.46055500

Cis-U-M8-M8

U	0.03759800	-1.12463300	-0.25408200
O	0.06753300	-2.22459000	-1.66498500
O	0.00170700	-0.24683400	1.29442900
O	2.40549400	-1.82458900	0.31648500
H	2.81518800	-0.91956200	0.19070600
O	-1.01951000	-3.05286900	1.00433500
C	-1.73856300	-2.96808500	2.27034700
C	-3.19611200	-2.59705100	2.07189700
H	-1.20477400	-2.20368600	2.83269400
H	-1.62232300	-3.92704700	2.78430800
H	-3.69426000	-2.54456000	3.04448300
H	-3.28972300	-1.62692100	1.57877600
H	-3.71949200	-3.35055100	1.47371600
C	3.19649000	-2.80105000	-0.38955600
C	4.47639700	-3.12111600	0.36704600
H	3.40975100	-2.43070700	-1.39736600
H	2.57071100	-3.68932900	-0.48852000
H	5.05026000	-3.88578800	-0.16515000
H	5.10603800	-2.23301200	0.46758000
H	4.24850500	-3.49203700	1.36886700

O	1.43740000	0.37406000	-1.16012400	C	-0.87674100	-1.64908900	-3.04931500
N	2.64730500	0.65645500	-0.54838500	C	-2.38614400	-1.79915300	-3.02290200
C	2.98374000	1.90669500	-0.61108500	H	-0.40183500	-2.25448800	-2.27884600
N	2.14612000	2.86518900	-1.12810600	H	-0.45037000	-1.92229800	-4.01921600
C	4.28348300	2.32941500	-0.04533800	H	-2.65380400	-2.83781600	-3.23863700
H	1.34656600	2.46798300	-1.60506200	H	-2.78752300	-1.52952900	-2.04347200
H	2.58320900	3.65222300	-1.58181900	H	-2.86094800	-1.17139600	-3.78445200
C	4.42242900	3.59437100	0.54178400	C	1.05951200	2.76841000	2.26315500
C	5.39492000	1.47717700	-0.09000200	C	2.57563000	2.80221100	2.20252300
C	5.64419300	3.99387000	1.07631300	H	0.68704400	2.99487300	3.26690600
H	3.56247800	4.25093700	0.60293500	H	0.61572700	3.47631800	1.56387300
C	6.61247200	1.87841400	0.44811200	H	2.93220800	3.79813500	2.48089000
H	5.29479700	0.50882100	-0.56362400	H	3.01689500	2.08378400	2.90018800
C	6.74234200	3.13815900	1.03235100	H	2.93121300	2.56857000	1.19813400
H	5.73502100	4.97185300	1.53552500	O	2.18726700	0.61049800	-0.65632700
H	7.46596900	1.21115700	0.40283800	N	3.02387700	-0.31826400	-0.04366200
H	7.69361800	3.45047000	1.44811300	C	4.26999300	-0.07158000	-0.29487900
N	-2.87434300	0.28645500	-0.09481900	N	4.69469300	1.03788800	-1.00640300
C	-3.81963500	0.75759300	-0.84587000	C	5.29086700	-0.98081100	0.27454500
O	-1.96244500	-0.46482000	-0.83168100	H	3.92129500	1.49324300	-1.47646600
N	-3.94485900	0.46171100	-2.18860000	H	5.51309300	0.90198400	-1.58137400
C	-4.85793500	1.60057900	-0.20910600	C	6.60559400	-0.54360600	0.48465900
H	-4.30974400	1.19859300	-2.77305700	C	4.95279000	-2.29779400	0.61921300
H	-3.12513400	-0.00778400	-2.55255700	C	7.56120400	-1.40408500	1.02064600
C	-6.14000100	1.70168500	-0.76549200	H	6.87325500	0.48116100	0.25511900
C	-4.57100400	2.31114100	0.96541200	C	5.90765300	-3.15082700	1.15807200
C	-7.11165000	2.49820300	-0.16396700	H	3.93624300	-2.63139900	0.45573600
H	-6.38388500	1.13269900	-1.65509300	C	7.21684000	-2.71001700	1.35816600
C	-5.54496300	3.10026700	1.56481600	H	8.57314000	-1.04905400	1.18179700
H	-3.57852700	2.23290100	1.39010600	H	5.63283800	-4.16721400	1.41797400
C	-6.81809500	3.20040300	1.00187700	H	7.96067200	-3.38004300	1.77467600
H	-8.10105200	2.56212500	-0.60329600	N	-3.10120700	-0.11225000	0.08864700
H	-5.30890400	3.64694500	2.47118000	C	-4.25494900	0.38882900	0.39919400
H	-7.57407200	3.82135900	1.46947000	O	-2.18540200	0.88089100	-0.24592300
H	-1.44129200	-3.70637100	0.43423500	N	-4.54961700	1.73563500	0.30504200

Trans-U-M8-M8

U	-0.00863400	0.66363700	-0.46089100	C	-6.67983400	-0.18994500	0.65751200
O	0.02481400	2.32379800	-1.13389900	C	-5.01620900	-1.79222300	1.36008500
O	-0.04215800	-0.99010900	0.20090800	C	-7.68872900	-1.06611500	1.05119200
O	0.52169600	1.47773000	1.86704800	H	-6.93717500	0.76019900	0.20415300
H	0.92279500	0.77837700	2.39769300	C	-6.02581100	-2.66513100	1.74641800
O	-0.45850900	-0.28561000	-2.74836400	H	-3.97385600	-2.05894300	1.47781400

C	-7.36607500	-2.30537800	1.59747600
H	-8.72730500	-0.78184400	0.92254200
H	-5.76773100	-3.62801700	2.17343400
H	-8.15130800	-2.98686300	1.90523600
H	-0.84911900	0.32285400	-3.38589200

Cis-U-M8-M9

U	-1.26847700	-0.43648400	-0.30249400
O	-0.96798600	-0.87448400	1.40011700
O	-1.70752300	-0.13731600	-2.01004500
O	-3.72864400	-1.34309100	-0.14217800
H	-4.13758200	-0.79898700	-0.82816500
O	-1.40737500	-2.97242600	-0.74569400
C	-0.45019000	-3.94048500	-0.24629300
C	-0.79267700	-4.40990600	1.15668900
H	0.50613000	-3.41832200	-0.26608300
H	-0.40739100	-4.77389200	-0.95479300
H	-0.03601300	-5.11686000	1.50853200
H	-0.82178000	-3.56253800	1.84375100
H	-1.76035800	-4.92331200	1.18111500
C	-4.47099300	-1.15508300	1.09628600
C	-5.92409100	-1.56401700	0.93687800
H	-4.36545700	-0.11367200	1.40711300
H	-3.95598200	-1.78081700	1.82493700
H	-6.44783900	-1.45768500	1.89088900
H	-6.43727000	-0.93041700	0.20666900
H	-6.00826200	-2.60379000	0.61191100
O	0.84632300	-0.67143900	-0.85285600
N	1.94675700	-1.14495200	-0.15582300
C	3.05809300	-0.71469700	-0.66270600
N	3.10724000	0.18788000	-1.71473300
C	4.33113500	-1.15635400	-0.04855300
H	2.20647100	0.25588700	-2.17513200
H	3.88378200	0.06669600	-2.34875300
C	5.51017400	-0.42126900	-0.23070000
C	4.37888500	-2.32186300	0.73041400
C	6.70762700	-0.84637700	0.34074000
H	5.48663600	0.50307000	-0.79554100
C	5.57319200	-2.74024700	1.30217600
H	3.46620900	-2.88351400	0.87896100
C	6.74510800	-2.00760600	1.10667200
H	7.60930800	-0.26220700	0.19354500
H	5.59345200	-3.64436000	1.90077800
H	7.67689000	-2.33865400	1.55138000

N	-1.43556600	1.89528600	0.21634900
C	-1.34704600	3.17402600	0.39133700
O	-2.67158100	1.31958300	0.31548000
N	-2.46072600	3.90384900	0.74718800
C	-0.03745900	3.84728400	0.27823400
H	-2.50748600	4.84419200	0.38523100
H	-3.31227800	3.36478800	0.65062400
C	0.16164000	5.11151200	0.85076500
C	1.03152300	3.23329200	-0.39059800
C	1.39449900	5.75008000	0.74444600
H	-0.63741800	5.58234300	1.41106800
C	2.26265300	3.86822900	-0.48406400
H	0.90028800	2.25253200	-0.82755100
C	2.44834900	5.13247300	0.07640500
H	1.53337500	6.72561200	1.19691500
H	3.07598900	3.36522400	-0.99409700
H	3.40955800	5.62814100	-0.00074900
H	-2.30527600	-3.31797800	-0.68128200

Trans-U-M8-M9

U	-0.35040400	0.78804400	0.31787300
O	0.03689600	0.63002000	-1.41484900
O	-0.71421800	1.03359200	2.05054400
O	0.20850400	3.27072700	0.24172800
H	-0.33993200	3.68536200	0.91932600
O	-0.74934000	-1.73183100	0.33370400
C	0.11970700	-2.67079700	-0.35565000
C	0.10002600	-4.02872900	0.32310400
H	1.11067300	-2.21887400	-0.32467300
H	-0.19328200	-2.73493900	-1.40233700
H	0.78713500	-4.70974800	-0.18731200
H	0.41408600	-3.94092600	1.36533600
H	-0.89805800	-4.47748200	0.29660200
C	0.09793900	4.03416400	-0.98958100
C	0.57333200	5.46233200	-0.79422800
H	-0.93689600	3.98740000	-1.33787700
H	0.72130100	3.49707900	-1.70314600
H	0.52371100	6.00502300	-1.74231700
H	-0.05440400	5.99683400	-0.07398900
H	1.60517300	5.48324900	-0.43713900
O	1.69407500	0.19279000	0.86406400
N	2.68416100	-0.39207300	0.08848200
C	3.84204700	-0.34232300	0.66863600
N	4.03003400	0.14757200	1.94688400

C	5.00825100	-0.90353000	-0.05090000
H	3.19942500	0.60815200	2.29812600
H	4.89345400	0.64366400	2.10903000
C	6.13458900	-1.35426000	0.65059900
C	5.00226000	-0.99324700	-1.45063100
C	7.23058900	-1.87824100	-0.03112700
H	6.13877200	-1.31977300	1.73376000
C	6.09532400	-1.52177900	-2.12609200
H	4.13152500	-0.64100100	-1.98847900
C	7.21582000	-1.96347200	-1.42066400
H	8.09257600	-2.22802500	0.52631600
H	6.07832300	-1.58274100	-3.20879600
H	8.06935200	-2.37041400	-1.95140200
N	-2.75495100	0.64129300	-0.10791400
C	-3.96182800	0.36870600	-0.48240900
O	-2.32512900	1.92280000	-0.23993800
N	-4.75637100	1.31760000	-1.09250800
C	-4.47061600	-1.00741400	-0.32012300
H	-5.74071800	1.28097900	-0.87226900
H	-4.34394600	2.24130300	-1.04596400
C	-5.33866200	-1.56358100	-1.26972300
C	-4.09728400	-1.77804800	0.79282000
C	-5.80419200	-2.86700200	-1.12075800
H	-5.62446100	-0.97729400	-2.13506900
C	-4.56029700	-3.08380100	0.93234700
H	-3.47600200	-1.33083900	1.56043300
C	-5.41351800	-3.63340700	-0.02437200
H	-6.46704100	-3.28816200	-1.86829000
H	-4.27082200	-3.66510300	1.80065500
H	-5.77851500	-4.64766100	0.08950500
H	-1.67162400	-1.99509800	0.22157100

Cis-U-M9-NO3-1

U	0.71861100	-0.02888200	-0.00686400
O	0.79484400	-0.28573700	1.74844100
O	1.29325400	-2.46005100	-0.34425000
O	-0.80819100	-1.98141900	-0.24304900
O	-0.18578400	-4.05818900	-0.50318800
N	0.08432000	-2.89411900	-0.37103300
O	0.77456100	0.20720700	-1.76346600
O	3.28038600	-0.38599300	-0.02744100
H	3.66160800	0.15438400	0.67471800
O	2.24099500	2.07663300	0.41999200
H	1.54554900	2.56954100	0.88044200

C	2.70237300	2.87550400	-0.70081700
C	3.41526400	4.13123200	-0.23028000
H	1.84926300	3.11088700	-1.34233700
H	3.37354000	2.21945700	-1.25487100
H	3.79380500	4.69081400	-1.09025500
H	2.73753700	4.78898100	0.32207100
H	4.25866000	3.88320400	0.41832100
C	4.13377400	-1.52579700	-0.30470700
C	4.36891000	-2.37829400	0.92859400
H	5.07252700	-1.14964100	-0.72406600
H	3.60867000	-2.08799000	-1.07371300
H	5.01432200	-3.22444300	0.67605500
H	4.86351700	-1.80781500	1.72167800
H	3.42326200	-2.76713600	1.30773200
O	-0.38330100	1.96597200	0.31250200
N	-1.41147100	1.06584700	0.19818500
C	-2.61685000	1.53857600	0.24045700
N	-2.82931900	2.89217300	0.32489900
C	-3.78085300	0.63475800	0.13847600
H	-3.66309700	3.19180800	0.80525200
H	-1.98940500	3.41838600	0.52337000
C	-4.99645900	1.11348900	-0.37136900
C	-3.69079500	-0.70308200	0.54490700
C	-6.10082000	0.27231300	-0.46591400
H	-5.06716600	2.13532700	-0.72528000
C	-4.79559900	-1.53985000	0.44124100
H	-2.75620400	-1.08541000	0.93065000
C	-6.00412500	-1.05608300	-0.05851700
H	-7.03261900	0.65243800	-0.86916300
H	-4.71017700	-2.57435500	0.75279200
H	-6.86353100	-1.71256000	-0.13502300

Cis-U-M9-NO3-2

U	0.86856600	-0.27053000	-0.03547600
O	0.84023100	-0.38040200	1.73801100
O	3.36817100	-0.32553100	-0.01746200
O	2.40410400	-2.23385500	-0.27726400
O	4.58569800	-2.12451900	-0.25065000
N	3.50606600	-1.59741700	-0.18696600
O	0.91989200	0.05892000	-1.78102200
O	1.96093200	2.05460100	0.43194900
H	1.80783600	2.29926800	1.35184300
O	-0.84363300	1.68621500	0.19734500
H	-1.71157600	1.27713300	0.31447700

C	-0.97064700	2.82068200	-0.69055500
C	-1.83569900	3.91019000	-0.07969600
H	-1.36706400	2.48437700	-1.65368000
H	0.04940900	3.16540600	-0.84807100
H	-1.88237600	4.77231300	-0.75129300
H	-2.85790800	3.55917000	0.08760500
H	-1.42486300	4.23991700	0.87722900
C	3.20862300	2.64459200	-0.02322200
C	4.30564100	2.53792100	1.01908100
H	3.00899600	3.68734300	-0.29215900
H	3.46981100	2.09319400	-0.92450000
H	5.21997200	3.00368800	0.64086200
H	4.02939100	3.05947900	1.94230900
H	4.51498100	1.49206100	1.24273400
O	-0.35269600	-2.16478400	-0.23486300
N	-1.36738600	-1.25537400	-0.20028700
C	-2.55417900	-1.72839500	0.02016000
N	-2.75241700	-3.05555400	0.29637200
C	-3.70760800	-0.80525400	0.03393300
H	-3.62038700	-3.46878400	-0.00676700
H	-1.92061900	-3.61977800	0.17335100
C	-4.73698500	-0.96513700	0.97212300
C	-3.79301400	0.23648000	-0.90179700
C	-5.81735400	-0.08838800	0.98571300
H	-4.67225500	-1.76411000	1.70127800
C	-4.87713800	1.11095100	-0.88306300
H	-3.02559700	0.32358600	-1.66197100
C	-5.89010200	0.95303900	0.06169100
H	-6.60215900	-0.21512900	1.72269600
H	-4.94221400	1.90226100	-1.62146700
H	-6.73615400	1.63049000	0.07089400

Trans-U-M9-NO3

U	0.84203800	0.03505500	-0.13348900
O	0.80947800	-0.03051500	-1.90213800
O	1.75692500	2.38191000	-0.26938900
O	2.48707100	-1.90835700	-0.02072800
O	3.22826400	0.80943300	-0.20316200
N	3.00129800	2.07072900	-0.25345300
O	3.87968100	2.89167300	-0.28272200
O	0.89572600	0.17019700	1.63596700
O	-1.04784500	1.76316400	-0.08329800
H	1.91239000	-2.68034300	0.06082500
H	-1.90751600	1.32980300	-0.00997300

C	-1.11999100	3.09063400	0.49847700
C	-1.43855700	3.04540900	1.98303600
H	-1.87001600	3.66048000	-0.05890000
H	-0.14356900	3.53124700	0.31182300
H	-1.44844100	4.06037800	2.39090800
H	-2.42151600	2.60131800	2.16884600
H	-0.68735600	2.46302500	2.51963300
C	3.69830100	-2.09278300	0.74879600
C	4.51942100	-3.24994400	0.20696000
H	3.43407400	-2.24266800	1.80075300
H	4.23250800	-1.14934000	0.65960100
H	5.44924100	-3.34684100	0.77458000
H	3.97895700	-4.19841800	0.28829600
H	4.77068100	-3.08370700	-0.84254400
O	-0.13585600	-2.05912000	0.02898400
N	-1.23052900	-1.26040200	-0.09837700
C	-2.39092700	-1.80737600	0.06794200
N	-2.51646400	-3.11816800	0.46065300
C	-3.60610900	-0.98466400	-0.10518500
H	-3.31921400	-3.62084000	0.11402300
H	-1.64060700	-3.62387300	0.43515500
C	-4.71742700	-1.17343600	0.72783400
C	-3.66556400	-0.01027200	-1.11374200
C	-5.85689700	-0.39078900	0.56647900
H	-4.67337500	-1.91789300	1.51403800
C	-4.80633400	0.77410200	-1.26510100
H	-2.82924200	0.10019900	-1.79414400
C	-5.90380400	0.58711300	-0.42573900
H	-6.70706100	-0.53931100	1.22246100
H	-4.84451600	1.51770500	-2.05299000
H	-6.79330300	1.19387300	-0.54985300

U-M11-M6

U	-0.09493200	0.20688900	0.25990300
O	0.95570500	0.07714400	-1.17925900
O	0.40233300	-2.13140600	0.70882400
O	2.47519000	-2.79138800	0.43673700
O	0.83302000	-4.07754000	-0.14378900
N	1.24047000	-3.02389500	0.30985700
O	-1.12688400	0.35664100	1.71108600
O	-0.99575400	2.43311800	-0.66673700
O	0.77053600	2.62503600	0.55058500
O	-0.05454800	4.39045100	-0.43865100
O	-1.89936300	-0.45374400	-0.80221500

N	-0.09806900	3.20199200	-0.19958600
O	1.88448900	0.32998600	1.58083500
N	3.00340400	-0.16811600	1.04553600
C	3.91054600	0.62440900	0.54538200
N	3.73829200	1.96568300	0.65461800
C	5.12796300	0.06791200	-0.07631200
H	4.18855800	2.52780500	-0.05017000
H	2.79438100	2.25964100	0.90475300
C	6.33467700	0.77752400	0.00394200
C	5.09459700	-1.15575700	-0.76124900
C	7.48811600	0.27301000	-0.58767900
C	6.25453000	-1.65533900	-1.34386700
H	4.16878800	-1.71277900	-0.84233200
C	7.45128300	-0.94502200	-1.26315200
H	6.21661800	-2.60118800	-1.87184500
H	8.35022200	-1.33876500	-1.72455500
N	-3.17024000	-0.62785800	-0.29457300
C	-4.21183500	-0.38189000	-1.18282200
N	-4.09293100	-0.18344000	-2.44071000
C	-5.56650800	-0.43413300	-0.55241100
C	-6.63185400	0.21085400	-1.19226700
C	-5.81106600	-1.11638800	0.64585600
C	-7.90653600	0.18932600	-0.63857500
C	-7.08967200	-1.13458500	1.20079100
H	-5.00453200	-1.65493900	1.12884800
C	-8.14064900	-0.48027400	0.56351800
H	-7.26383300	-1.67003400	2.12820700
H	-9.13566300	-0.49516800	0.99617400
H	8.41666700	0.82819300	-0.51392700
H	6.37045300	1.71198600	0.55182200
H	-6.42681400	0.71512900	-2.12818100
H	-8.72152600	0.69766300	-1.14366200
H	3.01006000	-1.20062500	0.94036800
H	-3.25921900	-0.20543200	0.62642200
H	-3.09619900	-0.15012600	-2.66524900

U-M12-M6

U	0.37615300	0.48101400	-0.17183400
O	-0.78263800	0.39887100	1.18434300
O	0.23992100	-1.95319700	-0.42236300
O	-1.74436900	-2.85087000	-0.17138500
O	0.02845800	-3.90952900	0.48330500
N	-0.49640200	-2.92723200	-0.01379900
O	1.50569300	0.57340200	-1.53973100

O	0.94671500	2.88503300	0.53464000
O	-0.72294800	2.72107300	-0.81732200
O	-0.17664300	4.67678200	-0.00958300
O	3.53947100	0.57179700	3.61833900
N	0.01389500	3.48173500	-0.08886100
O	-1.49017800	0.18408600	-1.63838400
N	-2.57411200	-0.38758800	-1.10595000
C	-3.59831000	0.33333600	-0.74201300
N	-3.58267500	1.66598500	-0.99727600
C	-4.77178600	-0.30172000	-0.11249800
H	-4.13355700	2.23979000	-0.37844600
H	-2.66752100	2.04669000	-1.23670700
C	-6.04995000	0.23355400	-0.32602600
C	-4.62645900	-1.42540800	0.71453400
C	-7.16379200	-0.34446200	0.27411700
C	-5.74685400	-2.00088500	1.30432200
H	-3.64451000	-1.84333700	0.90223900
C	-7.01526300	-1.46349100	1.09082700
H	-5.62276100	-2.86765700	1.94315900
H	-7.88322800	-1.91418300	1.55936300
N	4.07831000	0.12461600	2.52631000
C	3.41856300	-0.11955500	1.39339700
N	2.08599800	0.07013100	1.35622800
C	4.20374100	-0.67687100	0.27441700
C	3.69768700	-1.74007400	-0.48948900
C	5.48132500	-0.17849700	-0.02701200
C	4.46240900	-2.29798600	-1.50743000
C	6.24559400	-0.74768200	-1.04250400
H	5.85897700	0.68352700	0.51199200
C	5.74012500	-1.81123300	-1.78633100
H	7.22743000	-0.34341300	-1.26699000
H	6.32970100	-2.24811800	-2.58557300
H	-8.14787200	0.07538500	0.09751200
H	-6.16882100	1.08820600	-0.98185700
H	2.70859800	-2.12700500	-0.27687200
H	4.05502400	-3.11923900	-2.08717500
H	-2.46758500	-1.39331100	-0.88341200
H	5.06325200	-0.14234400	2.55303400
H	1.80171100	0.28450400	2.31720500

U-M11-M11

U	-0.01775800	1.12868400	-0.05642200
O	-0.75009500	1.29197800	-1.67754800
N	2.96402800	-0.12652400	-0.36474600

O	-0.89544500	3.49379400	0.60556600
C	4.13334800	-0.36907400	-1.00380900
O	1.92837200	0.50830900	-0.98384600
O	1.04809000	3.48026100	-0.33548200
N	0.10902500	4.15748100	0.19289700
O	0.16849000	5.37539900	0.29759400
O	0.73907600	1.00046800	1.55797000
N	-2.96420500	-0.16188600	0.22068600
O	-0.43298600	-1.37045000	-0.20405500
C	-4.24311200	-0.18284400	0.71508300
O	-2.07031800	0.67252300	0.85222000
O	1.28874300	-2.28813200	0.78696400
N	0.15902600	-2.40905800	0.26939200
O	-0.41220200	-3.49912100	0.19549200
N	-4.73192600	0.63940100	1.57939900
H	-3.96446300	1.24862500	1.87379700
C	-5.12721300	-1.23246300	0.11739600
C	-6.33538200	-1.53585500	0.75913400
C	-4.80980600	-1.91270000	-1.06577200
C	-7.19317000	-2.50181800	0.24481400
C	-5.66805300	-2.88458700	-1.57750000
H	-3.89708300	-1.66982300	-1.59588800
C	-6.86242000	-3.18564100	-0.92627400
H	-5.40070200	-3.40330000	-2.49275300
H	-7.52956900	-3.94281200	-1.32767100
N	4.48327300	0.19603200	-2.11796700
H	5.39639600	-0.16914200	-2.38306400
C	5.02134500	-1.32667300	-0.24874800
C	6.39659400	-1.06660000	-0.16504500
C	4.53043000	-2.50645300	0.32987100
C	7.25882400	-1.95182800	0.47433400
C	5.39732400	-3.39477100	0.96546200
H	3.47051200	-2.73381700	0.28752900
C	6.76214100	-3.12556400	1.04124700
H	4.99641600	-4.30339300	1.40337900
H	7.43172400	-3.81917500	1.54099400
H	-8.12383600	-2.72489800	0.75903900
H	-6.56965400	-0.98098000	1.65928600
H	6.77893900	-0.14794700	-0.59698000
H	8.31854600	-1.72188600	0.53732700
H	2.65561200	-0.75077000	0.37281100
H	-2.52257300	-1.04678500	-0.02477800

U-M11-M8

U	-0.10938300	0.39912300	-0.05490100
O	-0.87633600	0.37968500	-1.66796800
N	3.11817100	0.28520100	-0.38554700
O	-1.60849900	2.46209000	0.61542300
C	4.29136200	0.46160600	-1.03876200
O	1.92076400	0.52168300	-0.99581300
O	0.26568200	2.99894400	-0.30375600
N	-0.81843700	3.38504700	0.22247800
O	-1.10265000	4.56975700	0.34970100
O	0.63824000	0.49274000	1.56534500
N	-3.16767600	-0.95028700	0.39301100
O	0.42368400	-2.03098900	-0.21827900
C	-4.21121100	-0.21580800	0.63001600
O	-2.01156100	-0.44359300	0.86705100
O	2.33240700	-2.25268600	0.83440600
N	1.38427900	-2.76922200	0.19550500
O	1.35238800	-3.97853800	-0.04147200
N	-4.17649700	0.97879900	1.36747400
H	-3.20526700	1.23494800	1.52936600
H	-4.63156100	1.74186900	0.87825000
C	-5.51757300	-0.70963600	0.16363200
C	-6.71545200	-0.14405800	0.63292600
C	-5.60538700	-1.75885200	-0.77188400
C	-7.95212300	-0.60397800	0.18194900
C	-6.83850900	-2.21645700	-1.21256600
H	-4.68100200	-2.19155100	-1.13263300
C	-8.02512400	-1.64128800	-0.74354600
H	-6.87905200	-3.02511000	-1.93655400
H	-8.98757600	-1.99759800	-1.09821500
N	4.41098000	1.11177600	-2.15546700
H	5.39065500	1.08327400	-2.43253600
C	5.46709200	-0.13058000	-0.30060500
C	6.67327000	0.58292200	-0.25007400
C	5.42098300	-1.40281200	0.28921900
C	7.80135500	0.04840900	0.36441500
C	6.55485400	-1.93853600	0.89927700
H	4.49976300	-1.97649100	0.27915400
C	7.74855900	-1.22124000	0.93975900
H	6.49812200	-2.92666100	1.34495700
H	8.62704000	-1.64316700	1.41902500
H	-8.86287300	-0.15001600	0.56290900
H	-6.66432800	0.64375300	1.37505000

H	6.70918100	1.57394000	-0.68975200
H	8.72070300	0.62592200	0.40084200
H	3.04819200	-0.41252400	0.34920900

U-M12-M12

U	0.08980500	-0.10118700	0.07025900
O	0.17622800	-0.24798600	1.82862400
N	3.54824800	1.51395600	1.74615200
O	-0.16981800	-2.68247900	-0.41342400
C	3.47666100	0.98595000	0.51870500
O	2.59848200	1.98852100	2.47341200
O	1.86447600	-2.00404800	-0.21406100
N	1.05960400	-2.96380000	-0.47741300
O	1.46957200	-4.07867200	-0.77616000
O	0.10383400	0.03030900	-1.71151700
N	-3.41481400	-1.59305800	1.51072600
O	-0.67768800	2.22071000	0.18244200
C	-3.43003000	-0.77333900	0.45200200
O	-2.38295600	-2.10297200	2.09529100
O	-2.16297600	2.44123800	-1.41478100
N	-1.42491100	2.96676800	-0.55502100
O	-1.39607700	4.18660000	-0.37780700
N	-2.30768700	-0.35606900	-0.14196200
C	-4.78244300	-0.34314700	0.02277300
C	-4.97410200	0.92968800	-0.55121100
C	-5.90951200	-1.18377800	0.13655500
C	-6.23942800	1.34736200	-0.94920400
C	-7.17448300	-0.75350300	-0.25117800
H	-5.78389100	-2.19972700	0.49426600
C	-7.35240900	0.51873300	-0.79543200
H	-8.02134200	-1.42743100	-0.15357900
H	-8.33678700	0.85065000	-1.11141400
N	2.32417200	0.84321200	-0.15604200
C	4.77842000	0.52858300	-0.02448800
C	4.85335700	-0.67711500	-0.74989900
C	5.96099100	1.27797400	0.13401600
C	6.06612800	-1.11765300	-1.26716200
C	7.17383700	0.82514500	-0.37915300
H	5.91568900	2.24051900	0.63212700
C	7.23623200	-0.37531300	-1.08550200
H	8.06953300	1.42626800	-0.24775000
H	8.17914200	-0.72359700	-1.49623600
H	-6.35400800	2.33607900	-1.38316800
H	-4.12254000	1.58801600	-0.68715100

H	3.95635500	-1.27779500	-0.85911300
H	6.09979100	-2.05839800	-1.80842200
H	-2.52326200	0.18295300	-0.97520200
H	2.53577100	0.66080400	-1.13157600
H	-4.32351300	-1.73991100	1.95447200
H	4.47083200	1.42640600	2.18274700

U-M12-M8

U	0.06873800	0.75004200	-0.36803600
O	-0.45534300	0.72715200	1.32695300
N	-3.29150000	0.28904700	-0.43928200
O	1.18236600	3.09782300	-0.22298000
C	-3.74344200	-0.90175500	-0.18667700
O	-2.05597300	0.31632900	-0.97681900
O	-0.92853000	3.11470500	-0.66736900
N	0.14516400	3.77912300	-0.49099300
O	0.17063600	5.00003000	-0.57791400
O	0.55411600	0.77108600	-2.08642700
N	3.31705700	0.66126100	2.12714700
O	-0.06056500	-1.76973700	-0.45256500
C	3.36846100	0.04030300	0.94217400
O	2.37080400	1.40928300	2.58632400
O	1.68414900	-2.47192600	-1.57438400
N	0.62071100	-2.72742400	-0.98255400
O	0.18203200	-3.87939100	-0.88080500
N	2.37893900	0.11852600	0.04524300
C	4.59379300	-0.76719700	0.72775100
C	4.53684100	-1.96499000	-0.01223300
C	5.85121800	-0.36298500	1.22233900
C	5.67903000	-2.73370000	-0.20866100
C	6.98704300	-1.14396200	1.03220800
H	5.94378900	0.59361900	1.72467500
C	6.91104600	-2.33904400	0.31670000
H	7.94223800	-0.80242700	1.42178800
H	7.79918300	-2.94268100	0.15594900
N	-3.06332600	-2.08545100	-0.48193000
C	-5.11071100	-0.99980400	0.35650700
C	-5.80847900	-2.21980900	0.35029300
C	-5.75946600	0.12660800	0.89860600
C	-7.09935800	-2.31274700	0.86959400
C	-7.04575100	0.03007000	1.40897500
H	-5.22007100	1.06512400	0.90153500
C	-7.72845400	-1.19182500	1.40377200
H	-7.52215700	0.91364200	1.82415500

H	-8.73223500	-1.26402000	1.81167100
H	5.60141400	-3.65505600	-0.77796800
H	3.58912500	-2.28993000	-0.42871100
H	-5.33759100	-3.08921900	-0.09285800
H	-7.61605300	-3.26840100	0.84909300
H	2.65727800	-0.33468000	-0.81917400
H	-3.11349000	-2.76778600	0.26487300
H	-2.08389500	-1.91079800	-0.70569500
H	4.07906400	0.42536400	2.76637900

U-M14-M6

U	-0.04120900	0.58964700	0.34770500
O	0.80873600	-0.02022300	-1.09275700
O	0.16965700	-1.64291200	1.17291100
O	2.05293600	-2.71614800	0.88417700
O	0.19720500	-3.56032000	0.14769400
N	0.80893700	-2.67181300	0.70611000
O	-0.85493300	1.20124000	1.79118100
O	-0.72648700	2.62839700	-1.02037000
O	1.16908100	2.80366000	-0.01427300
O	0.49537900	4.41113300	-1.33350700
O	-2.00566500	-0.21617600	-0.68109000
N	0.31309700	3.33245600	-0.81768800
O	2.02929500	0.65537300	1.47037800
N	3.02494700	-0.12046800	1.02324600
C	4.00959200	0.39651700	0.33964000
N	4.04043500	1.73746800	0.15850800
C	5.09629300	-0.45995400	-0.17536200
H	4.54877600	2.07211500	-0.64402000
H	3.17469300	2.23012400	0.37223600
C	6.39936500	0.05097600	-0.25905300
C	4.84256000	-1.77318500	-0.59674900
C	7.43214700	-0.73753900	-0.75504900
C	5.88322300	-2.55572500	-1.08624700
H	3.84064400	-2.18274200	-0.54538600
C	7.17639800	-2.04271700	-1.17043800
H	5.67633400	-3.56882500	-1.41088300
H	7.98134900	-2.65770500	-1.55720700
N	-3.40140300	0.02067200	-0.27521800
C	-4.12202800	-1.06770300	-0.60071900
N	-3.76561900	-2.23824500	-1.07971000
C	-5.59809600	-0.82877200	-0.40366700
C	-6.48835800	-1.88955400	-0.60130900
C	-6.11056900	0.41928900	-0.02734700

C	-7.85819400	-1.70944400	-0.42895300
C	-7.48045500	0.59586100	0.15315300
H	-5.42210600	1.24144800	0.11825300
C	-8.36173000	-0.46590600	-0.04848700
H	-7.86155500	1.56865800	0.44875200
H	-9.42950800	-0.32514800	0.08945600
H	8.43725300	-0.33464300	-0.80921100
H	6.60444100	1.05671200	0.08894200
H	-6.06707800	-2.84368400	-0.89248700
H	-8.53541300	-2.54315500	-0.58928800
H	2.88079200	-1.13709700	1.14980700
H	-2.76334300	-2.39785900	-0.97469200
H	-2.01932200	-0.79131100	-1.47114300

U-M15-M6

U	-0.27744000	1.02058000	0.42895700
O	0.31831800	0.20816500	-1.03797500
O	-0.07863400	-1.19765400	1.66030500
O	1.23439700	-2.82584200	1.06268900
O	-0.91110200	-3.14657800	1.16611000
N	0.06533900	-2.41065800	1.27812100
O	-0.72985700	1.90119600	1.89913800
O	-0.31735800	3.22522900	-0.98591400
O	1.59248200	2.88617600	-0.07170400
O	1.34763800	4.55438500	-1.46097700
O	-2.38768000	1.85858200	-0.76939500
N	0.89533500	3.59666900	-0.86419500
O	1.91471700	0.66516200	1.35996500
N	2.63644400	-0.35746000	0.90572700
C	3.67961700	-0.14036000	0.15088400
N	4.03879800	1.14505600	-0.10252500
C	4.49210100	-1.25949200	-0.36496000
H	4.53113400	1.30106700	-0.96793800
H	3.32472000	1.83860300	0.12297500
C	5.87098600	-1.08257700	-0.55267500
C	3.90886600	-2.49264300	-0.69141400
C	6.65231700	-2.11765700	-1.05579100
C	4.69942100	-3.52402000	-1.18741400
H	2.84501900	-2.64606500	-0.55805100
C	6.06864100	-3.34187100	-1.37515500
H	4.23663800	-4.47223500	-1.43591600
H	6.67706400	-4.14943400	-1.76743300
N	-3.52779200	1.02887000	-1.10394100

C	-3.37668800	-0.06152800	-0.39701000
N	-2.30302900	-0.28536000	0.37323400
C	-4.48233800	-1.05875900	-0.52620100
C	-4.24639900	-2.41856000	-0.28756000
C	-5.77163300	-0.65413100	-0.89886200
C	-5.27743300	-3.34754300	-0.41276000
C	-6.79754500	-1.58442700	-1.02640800
H	-5.94740600	0.39779800	-1.08397900
C	-6.55623300	-2.93655900	-0.78121200
H	-7.79103600	-1.25309000	-1.31184700
H	-7.35830200	-3.66158600	-0.87553600
H	7.71816400	-1.96948800	-1.19046000
H	6.33005000	-0.13955100	-0.27969800
H	-3.25181900	-2.75371800	-0.01576700
H	-5.07535100	-4.39678400	-0.22431000
H	2.28304900	-1.30764500	1.12249500
H	-2.33215500	2.52581300	-1.46014800
H	-2.34639500	-1.13668300	0.91795400

U-M14-M14

U	-0.41155400	0.24450800	0.40671100
O	-0.96182300	0.29315600	-1.28477600
N	3.13339500	0.04692700	-0.21234800
O	-1.46503100	2.51437100	0.85116500
C	3.96262100	-0.37125200	-1.17547800
O	1.75314500	-0.03524400	-0.70602500
O	0.51823800	2.60382500	0.00897700
N	-0.49946700	3.24024400	0.43799700
O	-0.54910700	4.45637100	0.45255900
O	0.31391000	0.25509200	2.02381300
N	-2.65170600	-0.28743300	1.03354500
O	-0.30467300	-2.17605000	0.36108200
C	-3.97499500	-0.13946500	0.68593400
O	-2.54345200	-0.37757700	2.47584200
O	-1.09245700	-2.78609600	2.31730700
N	-0.51407200	-3.09070300	1.25510700
O	-0.14308300	-4.23419000	1.01669100
N	-4.98194600	0.03169800	1.48074100
H	-4.61119400	0.04967700	2.43248000
C	-4.27870800	-0.22171000	-0.78200000
C	-5.34447800	0.52900800	-1.29310700
C	-3.59857800	-1.09120800	-1.63989500
C	-5.71166700	0.42761600	-2.63091700
C	-3.97072200	-1.19888800	-2.97882300

H	-2.77623700	-1.67939600	-1.25620900
C	-5.02434500	-0.43922000	-3.48176600
H	-3.42679900	-1.87541800	-3.63029500
H	-5.30616600	-0.51876700	-4.52791300
N	3.75210100	-0.86211700	-2.38231300
C	5.40498400	-0.18668100	-0.77096900
C	6.41573000	-0.58836100	-1.65186700
C	5.77406000	0.37116900	0.46063000
C	7.75908800	-0.43703200	-1.31517600
C	7.11760700	0.51472000	0.80006700
H	4.98957200	0.68637700	1.13637700
C	8.11910600	0.11404700	-0.08545000
H	7.38430800	0.94493200	1.76150000
H	9.16631400	0.22980500	0.18071400
H	-6.53404200	1.02631800	-3.01266500
H	-5.87867900	1.17522700	-0.60784400
H	6.09997500	-1.01796500	-2.59486000
H	8.52910200	-0.75289900	-2.01448400
H	-2.07786300	-1.22942500	2.58199800
H	2.76987200	-1.11464200	-2.49129500
H	1.76317000	0.22535900	-1.64417300

U-M14-M8

U	0.06300200	0.65031100	-0.15635500
O	-0.66441500	0.72959900	-1.77349300
N	3.38238000	0.53100500	-0.68402000
O	-1.26455300	2.72518500	0.56504500
C	3.94587900	-0.63619500	-0.63056300
O	2.07875200	0.50055900	-1.05977600
O	0.66074100	3.12211000	-0.32605900
N	-0.40528900	3.59067700	0.19973600
O	-0.58336800	4.78748000	0.34138600
O	0.77034500	0.57670000	1.47378300
N	-3.17173000	-0.60397900	0.10774400
O	0.37728000	-1.81682800	-0.28918200
C	-4.23175800	-0.46368500	0.92386800
O	-1.93667700	-0.31562100	0.88912600
O	-0.49913600	-2.63307000	1.54292700
N	0.34882900	-2.71932600	0.63832600
O	1.16047100	-3.64544100	0.58169700
N	-4.35889300	-0.14859000	2.18922200
H	-3.42812500	0.05356800	2.55451700
C	-5.51546700	-0.75750900	0.17810100
C	-6.73084900	-0.70853600	0.87107800

C	-5.53828500	-1.07911200	-1.18587000
C	-7.93554100	-0.97493100	0.22428200
C	-6.74406400	-1.34385800	-1.83372600
H	-4.59596200	-1.11266900	-1.71701100
C	-7.95026300	-1.29481200	-1.13409800
H	-6.74127000	-1.58895600	-2.89264800
H	-8.88919500	-1.50165700	-1.64131300
N	3.32731800	-1.83083800	-0.98880000
H	3.48095800	-2.58747400	-0.33300000
C	5.37419800	-0.67435700	-0.25089600
C	6.15209400	-1.81978100	-0.48118400
C	5.99229400	0.43612200	0.35169200
C	7.49772100	-1.85721700	-0.11800200
C	7.33371500	0.39691500	0.70538500
H	5.38927000	1.31742900	0.52826800
C	8.09831700	-0.75166500	0.47729400
H	7.78843000	1.26580800	1.17183300
H	9.14525300	-0.78106800	0.76325300
H	-8.86850800	-0.93150000	0.78124600
H	-6.67913800	-0.45207600	1.92257900
H	5.69732300	-2.67266600	-0.97030600
H	8.07805800	-2.75553300	-0.30754700
H	-1.63941000	-1.17713300	1.25142700
H	2.32439100	-1.71099400	-1.10994200

U-M15-M15

U	0.07632700	-0.26635000	0.00902800
O	0.05453100	-0.87909500	1.70329300
N	3.82272900	-0.08811800	2.08326000
O	-0.56345500	-2.58889700	-0.89789200
C	3.56806300	0.29058900	0.86273100
O	2.71996900	-0.32782200	2.89569300
O	1.55895700	-2.26098000	-0.71093100
N	0.61599000	-3.03955200	-1.07028300
O	0.82827800	-4.14024900	-1.55122200
O	0.15223100	0.30498000	-1.68369100
N	-3.75451900	-1.35121800	1.52438600
O	-0.30528200	2.02285300	0.73626600
C	-3.50590300	-0.54470800	0.53062500
O	-2.65124900	-1.94560100	2.13616700
O	-1.69218500	2.75714100	-0.79274900
N	-1.01304400	2.98042100	0.22493300
O	-0.97969000	4.08248100	0.77325800

N	-2.29263900	-0.20950000	0.00256000
C	-4.75573700	0.06041100	-0.04062900
C	-4.74276400	1.32564600	-0.64646300
C	-5.97766900	-0.62828200	0.03075600
C	-5.91401100	1.87543100	-1.16827600
C	-7.14207000	-0.07720200	-0.49112000
H	-5.98350100	-1.59738600	0.51261000
C	-7.11858300	1.18043900	-1.09843200
H	-8.07352600	-0.63374400	-0.43026600
H	-8.02742600	1.61035000	-1.50989200
N	2.34231000	0.45281200	0.28049500
C	4.80786600	0.54068900	0.06004700
C	4.80295100	0.40675200	-1.33573600
C	6.01007400	0.91535200	0.68210400
C	5.95496800	0.64636100	-2.08357800
C	7.15829200	1.15205900	-0.06409700
H	6.01231400	1.00627400	1.76068400
C	7.13887500	1.02389700	-1.45516100
H	8.07474800	1.44623500	0.44010500
H	8.03489000	1.21502700	-2.03830500
H	-5.87774600	2.85944400	-1.62599000
H	-3.82118600	1.89673500	-0.69252700
H	3.89506000	0.08396400	-1.83195900
H	5.92449800	0.52884500	-3.16266200
H	-1.83546100	-1.49035800	1.86460000
H	1.90288200	-0.22350400	2.37722200
H	-2.43451700	0.39889300	-0.79866600
H	2.45819800	0.98642300	-0.57511400

U-M15-M8

U	-0.10233600	-0.69660600	-0.41693300
O	0.34739300	-0.77571800	1.32043500
N	3.27853000	-0.32764900	-0.43836600
O	-1.24789300	-3.01165700	-0.19900500
C	3.75355400	0.85052400	-0.17142000
O	2.03117100	-0.31933400	-0.95606500
O	0.82671500	-3.08012800	-0.78654400
N	-0.24442800	-3.72051700	-0.53218700
O	-0.30450000	-4.93907000	-0.60555800
O	-0.63197700	-0.68131000	-2.12380100
N	-3.24286600	-0.29887100	2.45928000
O	0.10385700	1.78569200	-0.47314400
C	-3.27594200	0.05762900	1.20512400

O	-2.07551000	-0.92334600	2.90033400
O	-1.64342900	2.44133600	-1.61824300
N	-0.59212200	2.72786800	-1.02966200
O	-0.16264900	3.88331200	-0.94954600
N	-2.31140000	-0.10038800	0.25263600
C	-4.56544200	0.73590400	0.84253800
C	-4.61275600	1.71678500	-0.15932300
C	-5.75880500	0.40782900	1.50617100
C	-5.81693400	2.33948400	-0.48822100
C	-6.95716600	1.02960900	1.17449700
H	-5.71199100	-0.33887300	2.28839300
C	-6.99623900	1.99948000	0.17003400
H	-7.86888100	0.75190000	1.69700400
H	-7.93323200	2.48228100	-0.09315500
N	3.09693600	2.05040900	-0.43771700
C	5.12952100	0.91179300	0.36059600
C	5.85925800	2.11214800	0.34855200
C	5.75033700	-0.23236200	0.89597600
C	7.15663700	2.16907200	0.85672500
C	7.04343800	-0.17211300	1.39542500
H	5.18588300	-1.15591700	0.90272400
C	7.75849300	1.03050500	1.38465600
H	7.49893600	-1.06843800	1.80623800
H	8.76714200	1.07496300	1.78412400
H	-5.82469000	3.10074000	-1.26266000
H	-3.70078700	2.01477200	-0.66603900
H	5.40959500	2.99499600	-0.09012000
H	7.69940000	3.10983900	0.83254300
H	-1.37098800	-0.82272400	2.23532400
H	-2.68241200	0.20281100	-0.64232400
H	3.19209700	2.73290500	0.30364700
H	2.10912000	1.91654600	-0.65464000

U-M9-M13-T3

U	0.02310200	-0.71981500	-0.25405000
O	0.05733000	-0.87040900	1.52041600
O	-0.07635500	-0.35533600	-1.99810400
O	-0.78800100	1.70114700	0.08693600
H	-1.65112200	1.71938700	0.51997200
C	-0.73430900	2.72181700	-0.93711900
C	-0.90827700	4.10982200	-0.34567400
H	-1.48853200	2.50978100	-1.70056100
H	0.24469100	2.60142200	-1.39946900

H	-0.82090200	4.86593500	-1.13101800
H	-1.89306800	4.22247500	0.11789900
H	-0.14721700	4.30772900	0.41228900
O	-1.67931800	-2.25507900	-0.37763700
N	-2.40077700	-1.11354500	-0.19334200
C	-3.64679300	-1.25353100	0.12573300
N	-4.19357800	-2.49608600	0.35497900
C	-4.47432500	-0.04746700	0.32589500
H	-5.15322900	-2.62581100	0.07185200
H	-3.56235600	-3.24583800	0.09912500
C	-5.47606500	-0.02368800	1.30582800
C	-4.27089900	1.09375900	-0.46495800
C	-6.24209200	1.12205100	1.50293200
H	-5.63129900	-0.89796300	1.92676200
C	-5.03739600	2.23753000	-0.26162000
H	-3.53452400	1.05372900	-1.25853000
C	-6.02393600	2.25697000	0.72462700
H	-7.00670600	1.13017700	2.27152900
H	-4.88253200	3.10798300	-0.88983500
H	-6.62463100	3.14629800	0.87719400
N	3.16443200	-1.48177500	-0.17468600
C	3.30921100	-0.16075100	0.01324100
O	1.93393300	-1.94759000	-0.51729800
N	2.23316300	0.58517600	-0.03644400
C	4.68480300	0.32957300	0.28581700
H	2.40644500	1.53068900	0.28414700
C	5.55317800	-0.38488200	1.12137000
C	5.12527700	1.52587900	-0.29454000
C	6.83974800	0.08819700	1.36465600
H	5.20691600	-1.29377400	1.59912500
C	6.41136800	1.99476900	-0.04859900
H	4.46208400	2.07230700	-0.95534700
C	7.27199800	1.27697600	0.78084800
H	7.50091200	-0.46700800	2.02021500
H	6.74496200	2.91735400	-0.50983300
H	8.27349800	1.64447500	0.97327600
H	3.93885500	-2.03673200	-0.51483800

U-M9-M13-T2

U	-0.12693200	0.83269900	0.00303300
O	0.07415900	0.72299300	1.77464600
O	-0.21422500	1.19417800	-1.74014500
O	0.09820600	3.34228200	0.41023900
H	-0.15646000	3.47817000	1.33150900

C	-0.60051500	4.30650600	-0.42619700	U	-1.34812300	-0.40820300	-0.10151800
C	-0.29069300	5.73011000	-0.00171800	O	-1.23824400	-0.18501100	-1.86097200
H	-1.67003500	4.08636000	-0.38849900	O	-1.57615500	-0.62965600	1.65130400
H	-0.24754800	4.09995600	-1.43552600	O	-3.77229600	0.48147000	-0.18753400
H	-0.79061600	6.43516600	-0.67154800	H	-3.45772800	1.40189100	-0.26923300
H	-0.64733400	5.93051200	1.01367700	C	-4.72417400	0.39691100	0.89706900
H	0.78377800	5.92342500	-0.03649200	C	-5.99191800	1.17126600	0.57792800
O	-2.31200400	1.56199200	0.32040100	H	-4.25420200	0.75261500	1.81839000
N	-2.43923900	0.21745400	0.11558800	H	-4.93602500	-0.66659300	1.01539800
C	-3.62234700	-0.29766800	0.20690400	H	-6.71919800	1.05380100	1.38647200
N	-4.71781700	0.51386500	0.41353700	H	-5.78375200	2.23966300	0.46805600
C	-3.81566800	-1.75050600	0.02662200	H	-6.44170600	0.81039800	-0.34953100
H	-5.45827900	0.12173300	0.97541200	O	-1.15255700	-2.67599000	-0.38102900
H	-4.44540900	1.45676600	0.66307200	N	0.13979700	-2.31215700	-0.13681800
C	-5.07764300	-2.25412100	-0.31976500	C	1.04606100	-3.22610600	-0.26082700
C	-2.74974800	-2.64769400	0.19595800	N	0.72813100	-4.48289300	-0.72316100
C	-5.27500300	-3.62289000	-0.48026600	C	2.45407000	-2.90260300	0.04368600
H	-5.89925300	-1.57016200	-0.49651700	H	1.25672700	-5.25061400	-0.33760800
C	-2.95293500	-4.01179400	0.02756000	H	-0.27133400	-4.63211600	-0.78530800
H	-1.76482700	-2.27680500	0.45049100	C	3.49390800	-3.53532100	-0.65085200
C	-4.21437000	-4.50709600	-0.30447200	C	2.77059800	-1.97069200	1.04303400
H	-6.25611600	-3.99539700	-0.75289400	C	4.82163300	-3.23527700	-0.35861000
H	-2.12046100	-4.69359100	0.16054100	H	3.25636200	-4.24229500	-1.43704600
H	-4.36668600	-5.57331500	-0.42944500	C	4.09876700	-1.67251600	1.32804300
N	1.83891200	-1.73637900	-0.09519500	H	1.96813600	-1.50237200	1.59951300
C	2.78725300	-0.78497400	-0.10480500	C	5.12886300	-2.30327800	0.62983100
O	0.54413000	-1.36128600	-0.28479700	H	5.61651000	-3.72526300	-0.90957400
N	2.40442700	0.46611300	-0.15884700	H	4.33224100	-0.95878900	2.11042700
C	4.19751800	-1.24776000	-0.03423500	H	6.16321500	-2.07320900	0.85893300
H	3.17596600	1.11104300	-0.03342700	N	-0.60940800	2.78224900	-0.04067200
C	4.56862200	-2.30390200	0.80806800	C	0.62498400	2.25801800	0.01458700
C	5.17667500	-0.61985500	-0.81468500	O	-1.67349700	1.94932100	0.14595800
C	5.89435300	-2.72548000	0.86227200	N	0.73931500	0.95652000	0.10972500
H	3.82162000	-2.77222200	1.43806500	C	1.76028800	3.21337700	-0.05991000
C	6.49988000	-1.04436900	-0.75698200	H	1.69153900	0.63075600	-0.00579200
H	4.89174600	0.18580500	-1.48171400	C	1.71628000	4.32045700	-0.91734400
C	6.86217900	-2.09807000	0.08096200	C	2.89718400	3.00713900	0.73164500
H	6.17288600	-3.53730500	1.52448200	C	2.78710900	5.20823800	-0.97260100
H	7.24802400	-0.55672700	-1.37148000	H	0.85582800	4.46429100	-1.56005900
H	7.89432500	-2.42620700	0.12636300	C	3.96475600	3.89643000	0.67268500
H	2.06094700	-2.66679100	-0.42477700	H	2.93147500	2.15866200	1.40510600
				C	3.91234700	4.99948700	-0.17822200
				H	2.74723800	6.05622600	-1.64669700
				H	4.83687200	3.73147600	1.29499900

U-M9-M13-T1

H	4.74667300	5.68995400	-0.22495400
H	-0.75895500	3.73596300	0.26194000

U-M9-M13-T2'

U	-0.06295500	0.39112100	-0.08203000
O	-0.14927600	0.40037300	1.70334800
O	0.22379800	0.57045700	-1.83495800
O	1.47974000	2.39303200	0.21805600
H	1.48783500	2.79220000	1.09520900
C	2.02311000	3.31176300	-0.76409100
C	3.46457500	3.67103000	-0.45260900
H	1.38333400	4.19834800	-0.80629700
H	1.93378500	2.78111000	-1.71070100
H	3.86091700	4.32962200	-1.23045000
H	3.54648900	4.20051100	0.50222700
H	4.08601500	2.77443800	-0.40816700
O	0.44912800	-1.84921400	-0.14551800
N	1.68464700	-1.30164700	0.03489500
C	2.69954200	-2.10004100	-0.03200400
N	2.53447800	-3.42831900	-0.36661600
C	4.06164400	-1.57549100	0.18625600
H	3.15024200	-4.08111200	0.09505800
H	1.55754700	-3.69578600	-0.37575300
C	5.16072600	-2.16762700	-0.45122900
C	4.28008500	-0.48548600	1.04112700
C	6.44672100	-1.67588700	-0.24431100
H	4.99872900	-2.99701000	-1.12951000
C	5.56558900	0.00479200	1.24082400
H	3.43538600	-0.04437600	1.55501100
C	6.65437700	-0.58830300	0.60052400
H	7.28632900	-2.13923800	-0.75030100
H	5.72246200	0.84246100	1.91154400
H	7.65642300	-0.20795900	0.76370600
N	-3.13437300	1.39845700	0.03997200
C	-3.36077600	0.07343100	-0.04270100
O	-1.86450800	1.82898600	-0.21290000
N	-2.32175300	-0.70291100	-0.20161000
C	-4.76937600	-0.38009400	0.07674000
H	-2.53053000	-1.69032400	-0.11916900
C	-5.65216300	0.23416700	0.97468600
C	-5.22820600	-1.44114000	-0.71443800
C	-6.97055300	-0.20210700	1.07186300
H	-5.29327500	1.03231600	1.61366300

C	-6.54591900	-1.87419100	-0.61309900
H	-4.55348100	-1.90997700	-1.42155500
C	-7.42059600	-1.25572000	0.27915800
H	-7.64307100	0.27355600	1.77663500
H	-6.89225200	-2.69163600	-1.23515400
H	-8.44667500	-1.59630600	0.35860700
H	-3.85908800	2.04329900	-0.24872800

U-M9-M16-T3

U	0.04015800	-0.18317900	0.20264000
O	-0.18578200	-0.32871200	1.96643700
O	0.15438900	0.26914100	-1.52033800
O	-0.85584500	2.13756400	0.60580700
H	-1.18636100	2.30911000	1.49506500
C	-1.22009400	3.21605300	-0.29467700
C	-0.57636900	4.52744800	0.11618800
H	-2.31101000	3.29022100	-0.32279400
H	-0.86999000	2.88445200	-1.27124600
H	-0.84315500	5.31175800	-0.59750500
H	-0.91717200	4.84884000	1.10518700
H	0.51146300	4.43610100	0.13584200
O	-1.15693300	-2.08381500	-0.22252600
N	-2.15328000	-1.14719800	-0.21735800
C	-3.37107500	-1.58401000	-0.19654000
N	-3.64442200	-2.92629300	-0.09015500
C	-4.48781700	-0.61816400	-0.22835000
H	-4.46897400	-3.26305700	-0.56294400
H	-2.81859000	-3.50444500	-0.18022600
C	-5.68168800	-0.88798300	0.45391500
C	-4.37099700	0.57830400	-0.94991000
C	-6.73147400	0.02599300	0.42438100
H	-5.77281800	-1.80296400	1.02735100
C	-5.42197000	1.48863200	-0.97471200
H	-3.46053300	0.76837400	-1.50472600
C	-6.60527600	1.21676100	-0.28754500
H	-7.64677200	-0.19020700	0.96368400
H	-5.32678700	2.40432800	-1.54796600
H	-7.42559500	1.92499100	-0.31390400
N	3.03002600	-1.71675900	-0.60673900
C	3.29987500	-0.56896600	-0.04898200
O	1.63572200	-2.02879700	-0.30171800
N	2.36747800	0.21339200	0.54563200
C	4.73396500	-0.16034900	-0.11388000

H	2.77721100	0.86317100	1.20690800
C	5.75451500	-1.11943200	-0.13613000
C	5.07829400	1.19582600	-0.15227200
C	7.08766100	-0.72742400	-0.19138600
H	5.48459900	-2.16703400	-0.10512200
C	6.41373800	1.58631000	-0.20469800
H	4.29319400	1.94302200	-0.16292900
C	7.42256100	0.62600900	-0.22284700
H	7.86875600	-1.47959300	-0.20296400
H	6.66579100	2.64054500	-0.23920700
H	8.46289300	0.92950300	-0.26174100
H	1.41521900	-2.74975100	-0.89994000

U-M9-M16-T2

U	-0.06494800	1.00517500	0.21470800
O	-0.17297700	1.14059800	1.99028600
O	0.15043000	1.08562300	-1.55261400
O	0.66284500	3.41115600	0.31474700
H	0.50879500	3.84047200	1.16446700
C	0.70705200	4.39926700	-0.75097000
C	1.83781900	5.38872300	-0.54055300
H	-0.26542100	4.89626900	-0.80481100
H	0.84257300	3.81385800	-1.65895100
H	1.86898800	6.09865500	-1.37148300
H	1.70083300	5.96319000	0.38093200
H	2.79991400	4.87482000	-0.49011500
O	-2.20834900	1.83364400	-0.00418600
N	-2.39949100	0.48207200	0.02920200
C	-3.59863600	0.04126200	-0.17554600
N	-4.61830800	0.90133900	-0.50884700
C	-3.86253300	-1.41065400	-0.11884300
H	-5.53997300	0.65856800	-0.17914900
H	-4.35838500	1.87397300	-0.40427400
C	-4.85332400	-1.98205900	-0.92923000
C	-3.12965600	-2.23663800	0.74664400
C	-5.09854000	-3.35146800	-0.88156700
H	-5.40861100	-1.35437400	-1.61615800
C	-3.37371300	-3.60554200	0.78346600
H	-2.38396500	-1.79676500	1.39671700
C	-4.35896600	-4.16736300	-0.02833600
H	-5.86119000	-3.78266700	-1.52013700
H	-2.80091100	-4.23279500	1.45691800
H	-4.54998300	-5.23382900	0.00646700

N	1.32458100	-2.12918100	-0.34772100
C	2.27562000	-1.31584200	0.02128400
O	0.04501900	-1.48842700	-0.02474200
N	2.06504100	-0.05813700	0.47016400
C	3.65444000	-1.87808500	-0.09578500
H	2.85101100	0.29522900	1.00393200
C	3.88947300	-3.24924300	0.06539400
C	4.73593200	-1.03340400	-0.37169800
C	5.17852000	-3.76005200	-0.04334600
H	3.05093500	-3.89938700	0.27856700
C	6.02593100	-1.54643400	-0.47776400
H	4.55796500	0.02477300	-0.52504600
C	6.25154900	-2.91106200	-0.31252200
H	5.34803100	-4.82307100	0.08826200
H	6.85363700	-0.88107000	-0.69748500
H	7.25628700	-3.31084600	-0.39346700
H	-0.59964900	-2.02289800	-0.49964900

U-M9-M16-T1

U	1.23884800	-0.63315600	-0.09375600
O	1.25230400	-0.81116200	-1.86463700
O	1.45344300	-0.65036800	1.67689900
O	3.52422600	-1.74828700	-0.21785400
H	3.86874600	-1.79952700	-1.11745700
C	4.62029800	-1.61500700	0.72952100
C	5.42793700	-0.35362300	0.48285500
H	5.23656000	-2.51678200	0.66658200
H	4.13465600	-1.59295200	1.70411400
H	6.21844700	-0.26810600	1.23386400
H	5.90587400	-0.37335600	-0.50172700
H	4.78798300	0.52887100	0.54253900
O	2.38454200	1.35136100	-0.26180400
N	1.08405000	1.75601500	-0.10715100
C	0.84226900	3.02371000	-0.20529300
N	1.83698100	3.90385500	-0.55354700
C	-0.52895600	3.52865600	0.00715300
H	1.77875500	4.83307600	-0.16690800
H	2.75623300	3.48104800	-0.55400400
C	-0.97594600	4.67011100	-0.67223600
C	-1.39474000	2.88395900	0.90211700
C	-2.26444300	5.15399600	-0.46413600
H	-0.32142800	5.15956400	-1.38392800
C	-2.68159100	3.37090400	1.10359000
H	-1.04683200	2.01160000	1.44071700

C	-3.12067500	4.50698700	0.42365900
H	-2.60169000	6.03233400	-1.00269200
H	-3.33960900	2.87037000	1.80501300
H	-4.12309000	4.88587400	0.58719000
N	-1.33132500	-3.03013500	0.27404600
C	-1.85522100	-1.85072000	0.06603100
O	0.14011500	-2.88503400	0.21460700
N	-1.15769600	-0.70598900	-0.06566900
C	-3.34982400	-1.86526800	-0.00186300
H	-1.74018700	0.06349400	-0.37308700
C	-4.03191200	-2.97778400	-0.50995300
C	-4.08987100	-0.76641100	0.44931900
C	-5.42175900	-2.98590400	-0.56786200
H	-3.45742100	-3.82581500	-0.85870400
C	-5.48076500	-0.77655000	0.39021900
H	-3.57507500	0.09241100	0.86414200
C	-6.15142600	-1.88577100	-0.11975700
H	-5.93705200	-3.85143600	-0.96952700
H	-6.04067700	0.08082000	0.74718900
H	-7.23466300	-1.89268200	-0.16869300
H	0.43510000	-3.55445000	0.83930400

U-M9-M16-T2'

U	-0.09991300	0.23361900	0.18964400
O	0.06001100	0.42894400	1.95476400
O	-0.07218200	0.32020300	-1.59126200
O	1.19505200	2.42485900	0.09404500
H	1.45429000	2.82345300	0.93249000
C	1.74596600	3.17548800	-1.02050800
C	3.25940100	3.25762500	-0.95286800
H	1.28879500	4.17007600	-1.02769300
H	1.41098100	2.63323300	-1.90349200
H	3.63972700	3.80114100	-1.82213100
H	3.59020800	3.79393900	-0.05758400
H	3.70485000	2.26115300	-0.94588300
O	0.62169400	-1.91855800	0.20826800
N	1.82551500	-1.25873000	0.19038800
C	2.87651400	-1.98879200	-0.00229500
N	2.76945200	-3.33096700	-0.27307400
C	4.21389000	-1.36183600	0.01247600
H	3.51084100	-3.92455500	0.06556900
H	1.82900400	-3.68368600	-0.14678100
C	5.23170700	-1.84219200	-0.82267800

C	4.48726400	-0.28932100	0.87249600
C	6.49341100	-1.25440600	-0.80437700
H	5.02170400	-2.66012700	-1.50179200
C	5.74926000	0.29527100	0.88603300
H	3.70865100	0.05952400	1.53951200
C	6.75630000	-0.18453700	0.04839700
H	7.27010100	-1.62926200	-1.46131600
H	5.95398300	1.11661800	1.56377300
H	7.74092300	0.26872600	0.06558200
N	-3.33926000	1.57909800	-0.19083800
C	-3.41632700	0.29385500	0.02383800
O	-1.94988600	1.98904100	0.08254300
N	-2.35975000	-0.49154600	0.31443800
C	-4.79525000	-0.26888600	-0.09445100
H	-2.63444100	-1.41021600	0.64205800
C	-5.91522300	0.49611800	0.25330000
C	-4.98423300	-1.57506100	-0.56092600
C	-7.19453600	-0.03849500	0.14210800
H	-5.76495900	1.50568400	0.61304600
C	-6.26562000	-2.10846500	-0.66998600
H	-4.12541600	-2.16533400	-0.85979200
C	-7.37444800	-1.34267900	-0.31713100
H	-8.05372900	0.56181700	0.42053600
H	-6.39747500	-3.12005400	-1.03763500
H	-8.37238900	-1.75887600	-0.39962000
H	-1.90132300	2.84078100	-0.35996400

U-M13-M13-T2

U	0.02855900	0.27487200	0.16604700
O	0.02268600	-0.34700000	-1.49998100
O	-0.00323500	1.00924900	1.78712400
O	-0.34529600	2.68672900	-0.71505400
H	0.59703400	2.78553200	-0.94845900
C	-0.73566400	3.77600600	0.14851800
C	-0.68895400	5.10674500	-0.58406100
H	-0.09641100	3.78069100	1.03587300
H	-1.75082600	3.54083400	0.47111900
H	-1.03525700	5.91117500	0.07144200
H	0.33116400	5.34761800	-0.89755200
H	-1.32495400	5.08381300	-1.47198000
O	1.95304300	1.60783200	-0.42456700
N	3.16076300	0.98912400	-0.50039400
C	3.30728900	-0.24147400	-0.00071400
N	2.25825400	-0.82345700	0.53291900

C	4.66420900	-0.84219600	-0.08305800
H	2.48706800	-1.67420400	1.03245600
C	4.80381200	-2.19943100	-0.39982100
C	5.81124300	-0.07622300	0.16204400
C	6.06713600	-2.77626700	-0.47617800
H	3.91937200	-2.79147900	-0.60517400
C	7.07386600	-0.65726500	0.08349400
H	5.70891300	0.96539900	0.44343300
C	7.20478600	-2.00700700	-0.23597900
H	6.16444800	-3.82572400	-0.72964000
H	7.95477700	-0.05831100	0.28461300
H	8.18842500	-2.45894300	-0.29396800
N	-2.37679300	-1.83541400	0.60716400
C	-3.12917100	-0.80714700	0.17234900
O	-1.07887300	-1.57537500	0.93134000
N	-2.53454200	0.33740500	-0.04218000
C	-4.57191200	-1.08431300	-0.04835500
H	-3.13225900	1.00369100	-0.51722200
C	-4.99653900	-2.29790900	-0.60485400
C	-5.52741200	-0.12096700	0.29939900
C	-6.35270200	-2.54280800	-0.80226000
H	-4.25985200	-3.03320700	-0.90617100
C	-6.88115900	-0.36961400	0.09961700
H	-5.20459100	0.81259300	0.74583500
C	-7.29737900	-1.58114900	-0.45060200
H	-6.67040100	-3.48128900	-1.24213600
H	-7.61259600	0.37989900	0.37956800
H	-8.35277500	-1.77276100	-0.60725300
H	-2.80590100	-2.56907200	1.15663200
H	3.81811400	1.36656900	-1.16839900

U-M13-M13-T3

U	-0.04816100	-0.15265100	-0.17645900
O	-0.02294500	-0.65387000	1.53929300
O	-0.06153900	0.68181900	-1.75775500
O	-0.05408400	2.22907900	0.76038100
H	0.17799000	2.35373900	1.68649500
C	-0.03056200	3.48499400	0.04471200
C	1.36598000	4.07867400	-0.02288300
H	-0.73781900	4.17272800	0.52022500
H	-0.40049400	3.23754700	-0.94886500
H	1.34975300	5.01036900	-0.59539200
H	1.75294800	4.30866300	0.97525200

H	2.04771500	3.38275800	-0.51508800
O	-1.62397100	-1.70259400	-0.78964700
N	-2.94782400	-1.59589000	-0.50850000
C	-3.40218200	-0.41802800	-0.05354300
N	-2.51877500	0.51716800	0.18484000
C	-4.86769100	-0.29743900	0.15813400
H	-2.91561700	1.31590600	0.66481900
C	-5.52508500	0.89209300	-0.18094000
C	-5.60864700	-1.35548600	0.70064700
C	-6.89651100	1.01820700	0.01362500
H	-4.95829800	1.70661700	-0.61736600
C	-6.98140600	-1.22534400	0.89327100
H	-5.10058300	-2.26639800	0.99457400
C	-7.62839700	-0.04000700	0.55072700
H	-7.39631000	1.94033800	-0.26068400
H	-7.54374300	-2.04702100	1.32210900
H	-8.69693800	0.06031300	0.70351600
N	2.81821700	-1.64885100	-0.54371700
C	3.30952900	-0.49341300	-0.07648000
O	1.49636500	-1.71873700	-0.83517700
N	2.46051500	0.47642200	0.16275800
C	4.77709700	-0.43230000	0.14922800
H	2.89771400	1.25010200	0.64901600
C	5.46676600	-1.51875600	0.70329100
C	5.48840600	0.72668700	-0.18660600
C	6.84178000	-1.44669100	0.90982500
H	4.91758100	-2.40590400	0.99599500
C	6.86197000	0.79482500	0.02176100
H	4.96273700	1.56314100	-0.63274700
C	7.54248100	-0.29158500	0.56992100
H	7.36390300	-2.29003400	1.34736500
H	7.40360900	1.69357300	-0.25075600
H	8.61272000	-0.23652900	0.73335100
H	-3.54922600	-2.20345900	-1.04927800
H	3.40647800	-2.28864000	-1.06091900

U-M13-M13-T1

U	-0.02861200	-1.06173800	-0.01027700
O	0.08303800	-0.93593200	1.76439200
O	-0.16825800	-1.29229400	-1.77193200
O	-0.44812100	-3.54386700	0.29988400
H	-0.55917200	-3.82381100	1.21529200
C	-1.13839700	-4.45670300	-0.59022500

H 3.05533600 1.11049100 0.15573900

U-M13-M10-T3

U -0.00208400 -0.25702400 0.16105600
O -0.12005100 -0.43496900 -1.61690500
O 0.02010400 0.30387000 1.86113600
O -0.01197900 2.25252700 -0.45928300
H 0.27165200 2.35652400 -1.37535400
C 0.51091400 3.33359300 0.35107700
C 0.03459500 4.68628400 -0.14733100
H 1.60328900 3.27342600 0.36909000
H 0.15261500 3.12090700 1.35726200
H 0.41235100 5.47910700 0.50393300
H 0.39671700 4.88938300 -1.16011900
H -1.05632000 4.73838900 -0.15411200
O 1.56474700 -1.89457300 0.46570500
N 2.89450500 -1.72675900 0.27453100
C 3.35604200 -0.50555700 -0.00867900
N 2.47696400 0.46179500 -0.14396700
C 4.82598900 -0.35894200 -0.16493300
C 5.47299200 0.76910500 0.35554000
C 5.58063000 -1.33073100 -0.83495000
C 6.84840100 0.91900200 0.21321200
H 4.89593100 1.51331600 0.89257500
C 6.95723100 -1.17708400 -0.97455900
H 5.08215900 -2.18967700 -1.26873000
C 7.59388600 -0.05366100 -0.45159000
H 7.34072600 1.79100700 0.62838000
H 7.53080000 -1.93059900 -1.50204900
H 8.66560500 0.06485600 -0.56273600
N -2.95801700 -1.68061500 0.33901600
C -3.44793300 -0.51252900 0.10492700
O -1.64103400 -1.72784200 0.52102000
N -2.54179800 0.62938500 0.06907200
C -4.89304600 -0.33698700 -0.11267600
H -2.70545100 1.19235400 -0.76205800
C -5.74429100 -1.45672700 -0.17537100
C -5.46245600 0.93649200 -0.26069100
C -7.10670600 -1.29850800 -0.37714200
H -5.31089700 -2.44169100 -0.06267400
C -6.83305200 1.08997000 -0.46432100
H -4.84105300 1.82340900 -0.21115000

C -7.66176000 -0.02442200 -0.52393700
H -7.74417000 -2.17461500 -0.42299500
H -7.24944500 2.08522600 -0.57460600
H -8.72750000 0.09357000 -0.68322500
H -2.70463800 1.23584000 0.87137100
H 3.48625500 -2.43377100 0.68902600
H 2.90865300 1.30474400 -0.50435500

U-M13-M10-T1

U -0.00449700 -0.98300000 -0.29871500
O -0.38919500 -0.95183400 1.44219800
O 0.32821900 -0.91151600 -2.04519000
O 0.58512200 -3.46079900 -0.15846900
H 1.54313700 -3.38236900 -0.01785600
C 0.01995600 -4.51155300 0.65749200
C 0.39505300 -4.37349900 2.12338200
H 0.34596300 -5.47266800 0.24721600
H -1.05803400 -4.43242400 0.51318400
H -0.07499200 -5.17220300 2.70433700
H 1.47787800 -4.45101900 2.26188800
H 0.06419100 -3.41099100 2.51714700
O -2.17357600 -1.37895900 -0.71067000
N -3.24070500 -0.62664400 -0.44059000
C -3.00917200 0.63275700 -0.30691900
N -1.63727300 1.11558900 -0.45984800
C -4.10658500 1.56932200 -0.01420000
H -1.42683600 1.80155400 0.26096300
C -3.91428000 2.95844600 -0.04073900
C -5.38910100 1.08130100 0.29936600
C -4.96444900 3.83244800 0.23579300
H -2.94420500 3.37370600 -0.28922200
C -6.43046800 1.95481900 0.57241300
H -5.54303500 0.01061300 0.32264500
C -6.22605400 3.33671400 0.54411800
H -4.79141400 4.90251000 0.20691900
H -7.41042600 1.55777700 0.81318200
H -7.04278300 4.01549100 0.76139400
N 3.22135300 -0.53943600 0.12821700
C 2.84073500 0.74276700 0.08310200
O 2.26573000 -1.50711100 0.15972700
N 1.56065700 1.00926200 -0.03485900
C 3.91887400 1.76301700 0.15404800
C 5.12345700 1.58968600 -0.53987600

C	3.73102900	2.92160800	0.91865000
C	6.12211800	2.55669000	-0.46346300
H	5.26162300	0.71232500	-1.16075500
C	4.73140700	3.88515400	0.99158000
H	2.80841900	3.05134400	1.47291900
C	5.92925600	3.70502500	0.30134900
H	7.04667500	2.41812400	-1.01208700
H	4.57923400	4.77374800	1.59342400
H	6.70717600	4.45775100	0.35745700
H	-1.52528900	1.58196400	-1.35959800
H	1.40092400	1.99473400	-0.20702800
H	4.10618900	-0.79177800	0.54783300

U-M16-M10-T1

U	-0.00233700	-1.12177700	0.23859700
O	0.16365300	-1.53542800	1.96176400
O	-0.19909800	-0.83057800	-1.50703200
O	-0.06945500	-3.63646700	-0.18856000
H	-0.04747900	-4.15884900	0.62226800
C	-0.91139200	-4.30246400	-1.17658900
C	-2.30662700	-4.56627700	-0.64233300
H	-0.40563300	-5.22273700	-1.48319100
H	-0.92879400	-3.61792700	-2.02395200
H	-2.92099400	-5.02037800	-1.42479600
H	-2.28286200	-5.26086800	0.20376200
H	-2.77642900	-3.63456600	-0.32123500
O	-2.23621700	-1.17889500	0.44181300
N	-3.13185500	-0.21483600	0.19760900
C	-2.67271400	0.98639600	0.24411500
N	-1.25357600	1.17967000	0.53363200
C	-3.56056700	2.14062100	0.02509300
H	-0.82807700	1.80549600	-0.14708800
H	-1.13406500	1.61392500	1.44815100
C	-3.09103000	3.45709200	0.13883200
C	-4.91423100	1.94203200	-0.30513700
C	-3.94237900	4.54097900	-0.06923500
H	-2.05601100	3.65159400	0.39506500
C	-5.75663400	3.02356600	-0.51155700
H	-5.28224800	0.92854900	-0.39455500
C	-5.27708900	4.33077800	-0.39562700
H	-3.55638900	5.54977300	0.02475500
H	-6.79613200	2.84922600	-0.76620500
H	-5.93943500	5.17298900	-0.55948100

N	3.39963000	-0.77783400	-0.59046400
C	2.96973000	0.34711500	-0.09201100
O	2.37338200	-1.79709700	-0.33157200
N	1.73318700	0.53426400	0.42566100
C	3.96302100	1.46229600	-0.14188700
H	1.70050300	1.36954800	0.99830100
C	5.33494000	1.20759200	-0.02451800
C	3.53200200	2.78336800	-0.31063000
C	6.25121800	2.25319000	-0.06933100
H	5.66551000	0.18529900	0.10504000
C	4.45034900	3.82877200	-0.35406600
H	2.47451300	2.98770000	-0.43315400
C	5.81295000	3.56688100	-0.23142700
H	7.31058600	2.04337800	0.02842600
H	4.10223100	4.84643100	-0.49214600
H	6.52886100	4.38059500	-0.26303400
H	2.60825500	-2.49843600	-0.94637000

U-M16-M10-T3

U	0.01091800	-1.00539100	0.07749600
O	-0.20130600	-1.05105700	1.84394200
O	0.24764500	-1.18510400	-1.67711900
O	0.01029000	-3.56149700	0.22931400
H	-0.20391100	-3.87288500	1.11678200
C	-0.50751400	-4.49452600	-0.75958800
C	-1.99493300	-4.73928700	-0.58116400
H	0.07194700	-5.42033000	-0.68977600
H	-0.29187000	-4.02204400	-1.71726300
H	-2.35797400	-5.40249800	-1.37147900
H	-2.20410100	-5.22291500	0.37886500
H	-2.54141800	-3.79554800	-0.62558100
O	-2.27594300	-1.34838100	-0.21101000
N	-3.16874500	-0.33374500	-0.04008000
C	-2.69798700	0.92223500	-0.04334200
N	-1.39737900	1.08148700	-0.07078300
C	-3.69759200	2.01909000	0.00062400
H	-1.11987300	2.04796700	0.04956900
C	-3.49842700	3.17345600	-0.76754100
C	-4.84081400	1.92120400	0.80455000
C	-4.42922900	4.20631800	-0.73654300
H	-2.62445800	3.24739200	-1.40460200
C	-5.77003400	2.95738300	0.83143400
H	-4.98238100	1.04646200	1.42831300

C	-5.56726000	4.10083600	0.06182800
H	-4.26952600	5.09186900	-1.34088100
H	-6.64643000	2.87634000	1.46418800
H	-6.29027400	4.90803900	0.08649400
N	3.53412600	-0.79214900	0.04850900
C	3.02716500	0.40796500	0.11612500
O	2.43897400	-1.74265500	0.28749300
N	1.71040800	0.67531500	0.24693700
C	4.03396900	1.50788400	0.02044300
H	1.54641400	1.64028900	0.50711300
C	5.32086000	1.35238700	0.54942600
C	3.70043200	2.71406700	-0.60681500
C	6.24893900	2.38469300	0.45803400
H	5.57538300	0.41762000	1.03183100
C	4.63068500	3.74598800	-0.69732300
H	2.71577400	2.83144900	-1.04508100
C	5.90713700	3.58543100	-0.16288800
H	7.24061100	2.25417700	0.87718300
H	4.36079200	4.67242000	-1.19228000
H	6.63125600	4.38978200	-0.23063300
H	2.78826200	-2.56568300	-0.06602100
H	-4.10121500	-0.52346900	-0.38299400

U-M16-M16-T1

U	0.04717000	-1.02806400	-0.24073200
O	0.02710200	-1.47635800	-1.96461800
O	0.16446500	-0.91052100	1.52959100
O	0.28032300	-3.54356900	0.15582300
H	0.30598800	-4.11093200	-0.62311100
C	0.86586300	-4.23142200	1.29778600
C	2.32040900	-4.58874100	1.05464000
H	0.25720500	-5.11498800	1.51220500
H	0.75962200	-3.52637000	2.12070700
H	2.73584400	-5.07491300	1.94152100
H	2.42549600	-5.28536900	0.21635800
H	2.90306100	-3.68993300	0.84585700
O	2.54264800	-1.32953100	-0.39657100
N	3.42846000	-0.16530300	-0.11625100
C	2.69850200	0.91888200	-0.21930700
N	1.38058300	0.93834000	-0.48190400
C	3.46447100	2.18627300	-0.00426000
H	1.03475600	1.87637700	-0.64144600
C	2.85683800	3.27618500	0.62917800

C	4.79338700	2.30009700	-0.42852100
C	3.56090600	4.46112700	0.82570900
H	1.83918400	3.18669000	0.99224900
C	5.49389400	3.48595300	-0.23355600
H	5.26313300	1.45242900	-0.91013400
C	4.87998800	4.57027500	0.39177700
H	3.08107400	5.29567200	1.32455900
H	6.52069900	3.56546900	-0.57279300
H	5.42770100	5.49385100	0.54230500
N	-3.40791300	-0.91710000	0.40343100
C	-3.00085100	0.25100700	-0.00679400
O	-2.32143500	-1.87427300	0.14742300
N	-1.74886800	0.50384300	-0.45221900
C	-4.02980000	1.33015400	0.06441900
H	-1.69234000	1.38720000	-0.94553200
C	-5.38396100	1.04738600	-0.15083300
C	-3.64813900	2.64499500	0.35603000
C	-6.33316800	2.06189300	-0.08128100
H	-5.67538900	0.02954000	-0.37534200
C	-4.59999300	3.65841200	0.42538000
H	-2.60534200	2.86677600	0.55245500
C	-5.94496400	3.37012800	0.20483700
H	-7.37844800	1.83240000	-0.25609100
H	-4.29169900	4.67136300	0.65906600
H	-6.68634300	4.15967900	0.25628300
H	-2.56255800	-2.61965200	0.70501800
H	2.92773700	-1.71347200	-1.19259200

U-H2O-H2O

U	-0.00000500	0.00002200	0.04501400
O	-0.00017200	-0.00018300	-1.71925900
O	-2.23823400	-1.07637800	-0.02103000
O	-0.00057300	2.53425400	0.02069200
O	-2.23888200	1.07642200	-0.02186700
N	-2.94150600	-0.00022500	-0.06516100
O	-4.13594800	-0.00063100	-0.13846500
O	0.00020500	0.00013400	1.80308100
O	2.23872800	1.07656000	-0.02179200
O	0.00023500	-2.53421300	0.02072800
O	2.23853300	-1.07626400	-0.02162600
N	2.94154400	0.00012200	-0.06528000
O	4.13601800	-0.00004100	-0.13833200
H	0.78476100	2.96968000	-0.33108100

H	0.78675500	-2.96845200	-0.32990500
H	-0.78431300	-2.96911200	-0.33347700
H	-0.78627900	2.96926300	-0.33077100

U-H2O-H2O-cis

U	-0.00012100	0.22206500	-0.00000500
O	-0.00058000	0.28366500	-1.76140800
O	-2.46995000	0.06686000	0.01200200
O	-1.41272000	-1.80610500	0.01305300
O	-3.59784900	-1.80661100	0.03597100
N	-2.55280400	-1.22656600	0.02182700
O	0.00127200	0.28233000	1.76142300
O	2.46966200	0.06652400	-0.01070900
O	1.41250400	-1.80648100	-0.01421500
O	3.59759300	-1.80699300	-0.03603500
O	-1.36761400	2.42513900	-0.05882400
N	2.55247300	-1.22711300	-0.02188500
H	-1.25582700	2.92331400	-0.87719600
O	1.36864800	2.42515900	0.05894100
H	2.29783500	2.15538100	0.01615200
H	1.26186600	2.91962900	0.88026900
H	-2.29813200	2.15955600	-0.01996500

TS-M8-M9

U	0.13018600	0.92771200	-0.14848300
O	-0.60519000	0.83117500	1.47319200
O	0.78810100	1.14558400	-1.79428400
O	-0.71801400	3.28197500	-0.29196300
H	-0.74539200	3.64115200	-1.18642800
O	0.88543600	-1.48677200	0.03340100
C	0.40573400	-2.52235000	0.92050700
C	1.15753600	-3.82436800	0.70046300
H	-0.65204700	-2.63405000	0.68206300
H	0.49191900	-2.17954200	1.95637600
H	0.75458600	-4.60470000	1.35267000
H	1.05898000	-4.15521200	-0.33596100
H	2.22170300	-3.71302400	0.92710900
C	-1.76705500	3.88696700	0.51887100
C	-3.14570200	3.63573200	-0.06176100
H	-1.54306800	4.95384200	0.61171100
H	-1.65486700	3.42088900	1.49656900
H	-3.90177200	4.09160700	0.58458000

H	-3.24577100	4.08573300	-1.05530000
H	-3.34401900	2.56400400	-0.13554200
O	-1.75803400	0.26301000	-1.03993200
N	-3.01615100	0.09057000	-0.48693900
C	-3.45710600	-1.11646300	-0.63552700
N	-2.69238900	-2.14002200	-1.18060200
C	-4.81358300	-1.44092500	-0.13935300
H	-1.89156700	-1.77419000	-1.68307500
H	-3.21530600	-2.83046100	-1.70037000
C	-5.15009100	-2.75245300	0.22249300
C	-5.78806900	-0.43910200	-0.02561400
C	-6.42949600	-3.05476600	0.68308400
H	-4.40057400	-3.53353200	0.17118600
C	-7.06178900	-0.74375000	0.43752500
H	-5.52910600	0.57202000	-0.31081700
C	-7.39001900	-2.05317900	0.79135800
H	-6.67153900	-4.07348700	0.96507000
H	-7.80581100	0.04125400	0.51664900
H	-8.38624400	-2.28868400	1.14854100
N	2.84917600	0.44342300	0.38553200
C	4.12246400	0.56959600	0.58640100
O	2.10836000	1.54886800	0.77429200
N	4.65154300	1.66113800	1.23737800
C	5.02679800	-0.52598500	0.17402500
H	5.56823800	1.95811800	0.93939700
H	3.96964800	2.40110000	1.35384300
C	6.19663700	-0.79567300	0.89714200
C	4.73055800	-1.30424600	-0.95436800
C	7.04652300	-1.82645900	0.50480700
H	6.42377200	-0.21085800	1.78087900
C	5.57972200	-2.33599900	-1.33880900
H	3.84312400	-1.07777500	-1.53251900
C	6.74063100	-2.60065400	-0.61204500
H	7.94485300	-2.02894100	1.07722000
H	5.34249400	-2.92676500	-2.21650200
H	7.40404900	-3.40177400	-0.91776800
H	1.81393600	-1.23820600	0.23041900