

Electronic Supplementary Information

for

Predominance of the Second Cycle in the Homogeneous Os-Catalyzed Dihydroxylation: Nature of Os(VI)→Os(VIII) Reoxidation and Unprecedented Roles for the Amine-N-Oxide

Aqeel A. Hussein¹, Yumiao Ma^{2,3}, and Gamal A. I. Moustafa^{4,5}

¹ Department of Pharmacy, College of Medicine, Komar University of Science and Technology, Sulaymaniyah, Kurdistan Region, Iraq.

² BSJ Institue, Haidian, Beijing, 100084, People's Republic of China.

³ Hangzhou Yanqu Information Technology Co., Ltd. Xixi Legu Creative Pioneering Park, No. 712 Wen'er West Road, Xihu District, Hangzhou City, Zhejiang, Province, 310003, People's Republic of China.

⁴ Department of Medicinal Chemistry; Faculty of Pharmacy, Minia University, Minia 61519, Egypt.

⁵ Department of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, UK.

Email: aqeel.alaa@komar.edu.iq

TABLE OF CONTENTS

1	Simple hydrolysis of Os(VI) dioxoglycolate 11	2
2	Energetic comparison of hydrated forms of Os(VI) oxobisglcolate 17	3
3	The method-dependency of the energetics of TS 16	4
4	Comparison between Solvated and Gas-Phase Optimizatin on Ion-Pairing Hydrolysis Mechnaism of Interemdiates 11 _[ox] and 16	5
5	Absolute energies for the structures calculated in this study	6
6	Supplementary cartesian coordinates	9
7	References	34

1. Simple hydrolysis of Os(VI) dioxoglycolate **11**

We considered hydrolysis of Os(VI) glycolate **11** without the involvement of NMO or NMM (Figure S11). Without ligands, calculations show hydrolysis of Os(VI) glycolate **11** following an endergonic pathway, requiring substantial barriers to be overcome via TS's **12** and **14** ($\Delta G^\ddagger = 34.5$ kcal/mol and 19.9 kcal/mol, respectively) and with an unstable intermediate **13** ($\Delta G_r = 25.3$ kcal/mol) to release the vicinal diol **9** (Figure S11). These results explain the favorable coordination of the diol to Os(VI).

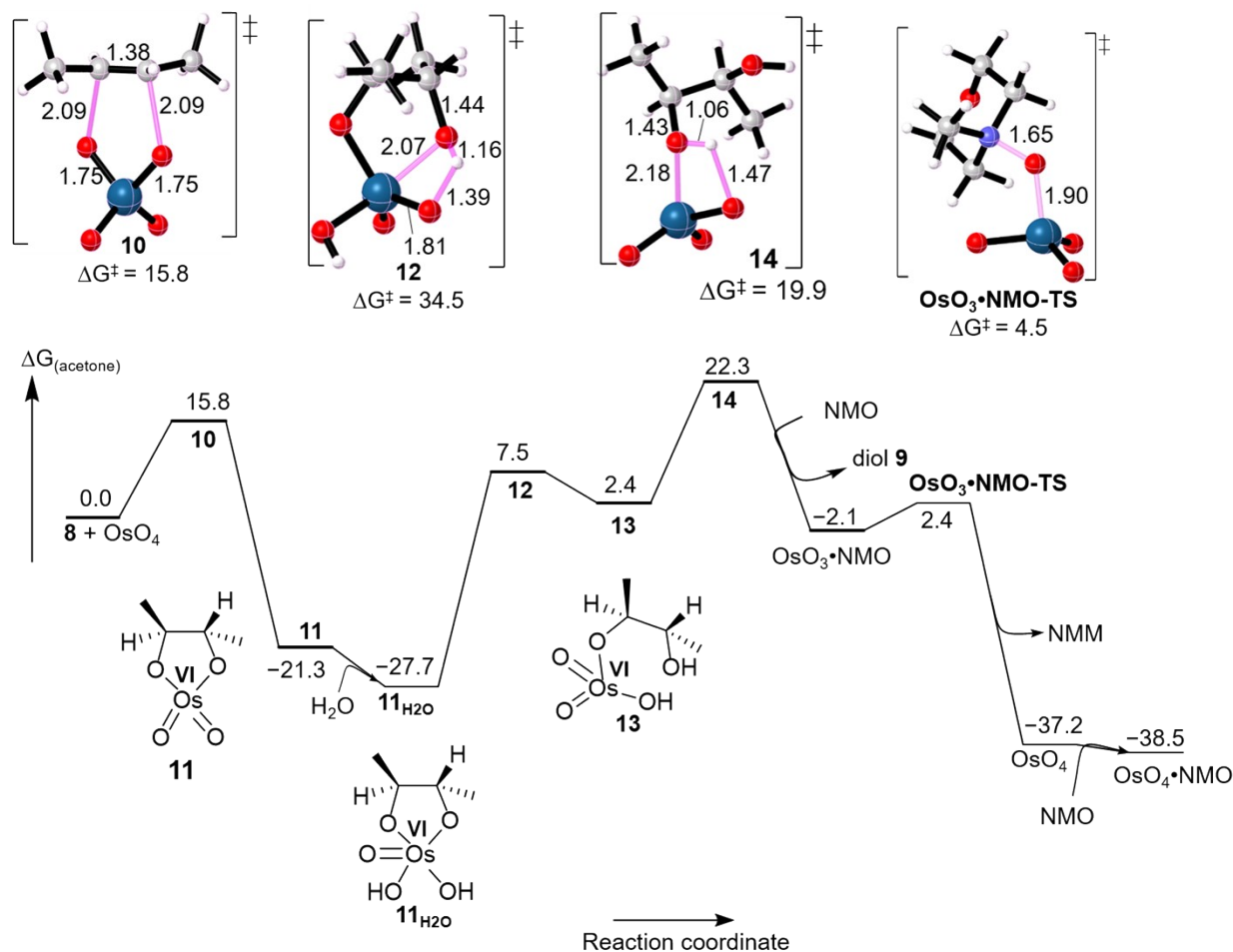


Figure S11. Formation and unfavorable hydrolysis of Os(VI) dioxoglycolate **11**

2. Energetic comparison of hydrated forms of Os(VI) oxobisglycolate **17**

Thermodynamic calculations for the formation of hydrate **17**_{H₂O} from Os(VI) oxobisglycolate **17** and isomerization to dihydroxybisglycolate **17**_{2(OH)} show the latter to be unstable under neutral conditions. Previous experimental efforts to isolate the conjugate acids of osmate bisglycolates (e.g. **17**_{2(OH)}) were reported to give the corresponding Os(VI) oxobisglycolates (e.g. **17**) instead.¹ The experimental results are consistent with the calculated instability of **17**_{2(OH)}.

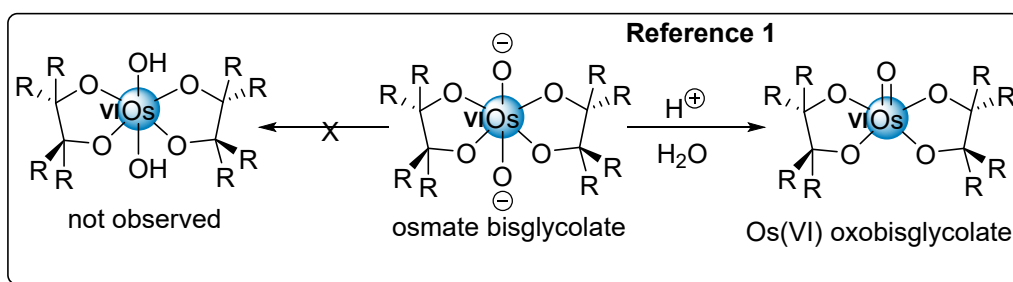
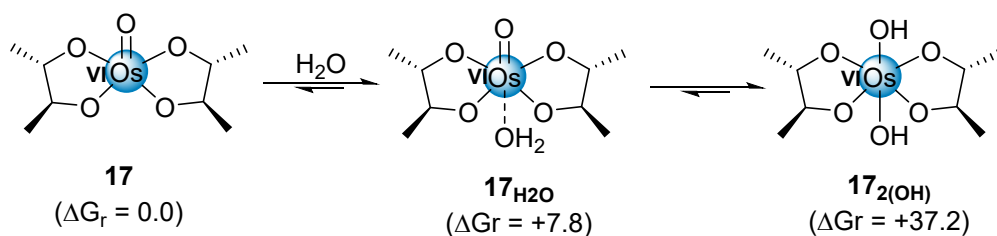


Figure S2. Thermodynamic calculations for hydration Os(VI) bisglycolate **17**.

3. The method-dependency of the energetics of TS 16

Table S11. Calculated relative Gibbs free energies of **16** with isolated butene and **11ox** as the zero point.

Level for opt+freq	Level for single point	Grel (kcal/mol)
PBE0-D3BJ/6-311+G(d,p)/def2-TZVP/SMD	PBE0-D3BJ/6-311+G(d,p)/def2-TZVP/SMD	TS does not exist
MN15/6-311+G(d,p)/def2-TZVP/SMD	MN15/6-311+G(d,p)/def2-TZVP/SMD	-2.2 ^a
M06/6-311+G(d,p)/def2-TZVP/SMD	M06/6-311+G(d,p)/def2-TZVP/SMD	-2.3 ^a
M06/6-31G(d)/LanL2DZ/gas	M06/6-311+G(d,p)/def2-TZVP/SMD	TS does not exist
M06/6-31G(2d)/LanL2DZ/gas	M06/6-311+G(d,p)/def2-TZVP/SMD	0.6 ^b
M06/6-311+G(d,p)/def2-TZVP/SMD	M06/6-311+G(d,p)/def2-TZVP/SMD	0.8 ^a

^a The geometries of **16** and **11ox** were re-optimized at the same level.

^b The geometries of **16** and **11ox** were optimized at M06/6-31G(d)/LanL2DZ/gas level.

4. Comparison between Solvated and Gas-Phase Optimization on Ion-Pairing Hydrolysis Mechanism of Intermediates $11_{[ox]}$ and 16

We have run optimization in solvent, and we have found that the solvation has a negligible influence on the energies as shown below for hydrolysis mechanism of intermediates $11_{[ox]}$ and 16.

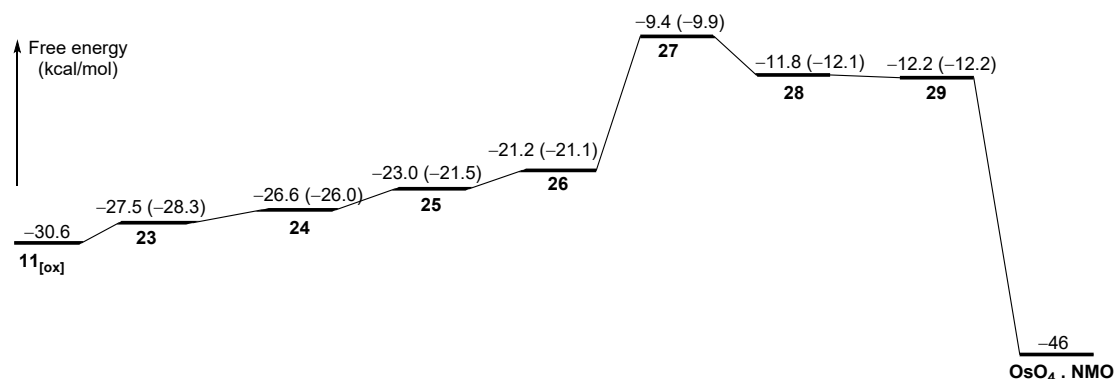


Figure S3. Comparison between Solvated and gas phase optimization of intermediate $11_{[ox]}$. The solvated results are shown in parentheses. The effect of solvated optimization is negligible when compared to gas phase optimization.

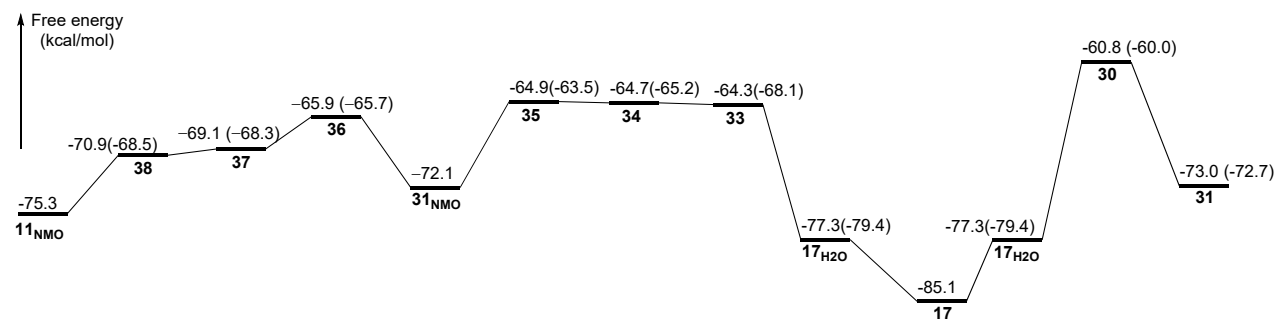


Figure S4. Comparison between Solvated and gas phase optimization of intermediate 17_{H_2O} . The solvated results are shown in parentheses. The effect of solvated optimization is negligible when compared to gas phase optimization.

5. Absolute energies for the structures calculated in this study

Table SI2. Absolute energies for the structures calculated in this study in Hartree units. “optSMD” means that the structure is optimized under SMD solvation of acetone.

Structure	E (M06)	G (M06)	Thermal Gibbs free energy correction
OsO₄	-391.546436962	-391.559873	-0.016448
OsO₄.NMO	-793.697235114	-793.550247	0.143976
OsO₃	-316.334654091	-316.350034	-0.018392
OsO₃.NMO	-718.488354065	-718.345866	0.139476
OsO₃.NMO.H₂O	-794.922675534	-794.760854	0.1588100
OsO₃.NMO-TS	-718.479449602	-718.338638	0.137800
OsO₃.NMO.H₂O -TS	-794.908340152	-794.742638	0.162690
OsO₃.2NMO-TS	-1120.632115230	-1120.332535	0.296568
NMO	-402.128191879	-401.988235	0.136945
NMM	-326.977191134	-326.841472	0.132707
NMM-H⁺	-327.436275209	-327.286562	0.146701
H₂O	-76.426612211	-76.420333	0.003267
(E)-2-Butene (8)	-157.129556569	-157.045891	0.080654
9	-308.795744666	-308.682577	0.110156
10	-548.669008987	-548.580592	0.085405
11	-548.734675508	-548.639746	0.091918
11TS	-625.14044139	-625.025551	0.111878
11TS_2	-701.58960340	-701.452000	0.134591
11_{H2O}	-625.190219640	-625.070222	0.116986
11_{NMM H2O}	-952.166586536	-951.889518	0.274057
11_{NMM}	-875.740103363	-875.488799	0.248292
11_{2NMM}	-1202.730171840	-1202.322198	0.404962
11_{NMO}	-950.899138748	-950.644494	0.251633
11_{2NMO}	-1353.029970180	-1352.615437	0.411521
11_{NMO NMM}	-1277.89928122	-1277.4853603	0.410909
11_[ox]	-623.897692192	-623.801349	0.093331
11_{[ox]NMM}	-950.878235763	-950.631799	0.243425
12	-625.131287110	-625.015194	0.113081
12_{NMM}	-952.139947733	-951.864945	0.271991
12_{NMM.H2O}	-1028.587912870	-1028.290735	0.294166
12_{NMO}	-1027.279731140	-1027.002692	0.274027
12_{H2O}	-701.588442754	-701.450447	0.134984
12_{NMO.H2O}	-1103.74653487	-1103.446538	0.296985
13	-625.150618680	-625.032445	0.115162

13 _{H2O}	-701.606191139	-701.463990	0.139189
13 _{NMO}	-1027.334083510	-1027.055799	0.275273
13 _{NMO.H2O}	-1103.773772880	-1103.472402	0.2983590
13 _{NMM}	-952.132437428	-951.860508	0.268918
13 _{NMM.H2O}	-1028.602895440	-1028.306449	0.293435
14	-625.112551526	-625.000686	0.108854
14 _{NMO}	-1027.283205230	-1027.007281	0.272912
14 _{NMO.H2O}	-1103.689778470	-1103.393254	0.293513
15	-950.875095649	-950.625077	0.247007
15 _{NMO}	-1353.011791250	-1352.598118	0.410661
15 _{NMM}	-1277.845713670	-1277.4346938	0.408008
16	-781.042672900	-780.846398	0.193263
17	-781.139123851	-780.934196	0.201916
17 _{H2O}	-857.568838033	-857.342036	0.22379
17 _{2(OH)}	-857.523427345	-857.295215	0.225200
17 _{NMO}	-1183.284103300	-1182.915685	0.365406
17 _[ox]	-856.226355605	-856.019442	0.203902
18	-700.308319824	-700.190000	0.115308
18 _{H2O}	-776.752334885	-776.611554	0.137769
19	-700.322313274	-700.199100	0.120201
19 _{H2O}	-776.763050170	-776.616964	0.143074
20	-700.297781754	-700.183119	0.111651
20 _{H2O}	-776.747321849	-776.608221	0.136089
21	-1107.975357610	-1107.6144097	0.357936
25	-1108.039656850	-1107.675234	0.3614110
23	-1027.333437750	-1027.058238	0.272188
24	-1027.334442830	-1027.056810	0.274621
25	-1027.325807180	-1027.051037	0.271758
26	-1027.328036950	-1027.048246	0.276779
27	-1103.748603	-1103.449772	0.295819
28	-1103.755921570	-1103.453724	0.299186
29	-1103.753497880	-1103.454174	0.296312
30	-857.542444910	-857.315681	0.223752
30 _{H2O}	-933.981794322	-933.731712	0.24707
31	-857.565217392	-857.335168	0.227037
31 _{NMO}	-1259.710925440	-1259.318049	0.389865
31 _{H2O}	-934.001661929	-933.746187	0.252463
32	-857.517157853	-857.292363	0.221783
32 _{NMO}	-1259.682856070	-1259.297159	0.382685
32 _{NMO.H2O}	-1336.129980160	-1335.720158	0.406810
33	-1184.546848350	-1184.162883	0.380953
34	-1184.551101950	-1184.163534	0.384556
35	-1184.548010170	-1184.163819	0.381179

36	-1586.69193677	-1586.149638	0.539287
37	-1586.70446291	-1586.154730	0.546721
38	-1586.70525185	-1586.157618	0.544622
H2O_optSMD	-76.42655382	-76.42052592	0.003016
17_optSMD	-781.13987655	-780.9356076	0.201257
11ox_optSMD	-623.89776130	-623.8019964	0.092753
NMM_optSMD	-326.97721447	-326.8423986	0.131804
23_optSMD	-1027.33234937	-1027.061326	0.268011
24_optSMD	-1027.33462925	-1027.057657	0.27396
25_optSMD	-1027.32372147	-1027.050357	0.270353
26_optSMD	-1027.32587127	-1027.049781	0.273078
27_optSMD	-1103.74780915	-1103.452472	0.292325
28_optSMD	-1103.75588162	-1103.455919	0.296951
29_optSMD	-1103.75158063	-1103.456154	0.292415
17H2O_optSMD	-857.57250096	-857.3470851	0.222404
33_optSMD	-1184.55115342	-1184.171513	0.376629
34_optSMD	-1184.55382211	-1184.166785	0.384025
35_optSMD	-1184.54686055	-1184.164082	0.379767
30_optSMD	-857.54266466	-857.3161628	0.22349
31_optSMD	-857.56548421	-857.3363053	0.226167
31NMO_optSMD	-1259.71100860	-1259.320278	0.387719
36_optSMD	-1586.69425690	-1586.152554	0.538691
37_optSMD	-1586.70661421	-1586.156582	0.547020
38_optSMD	-1586.70365893	-1586.157015	0.543632

6. Supplementary

OsO₄

O 0.21344600 -1.62926900 -0.44506200
O -0.78191500 0.07717600 1.50957700
O 1.51794400 0.76309700 0.10599200
O -0.95201900 0.78804400 -1.17063500
Os 0.00026800 0.00010000 0.00001300

OsO₄.NMO

Os -1.42293100 -0.09554300 -0.03810500
O -1.42334400 1.41066700 -0.85097800
O -0.77636000 -0.03758300 1.55641700
O -3.08781200 -0.36579000 0.25120000
O -0.99742700 -1.45583600 -0.98212800
C 2.84510100 -1.33952600 0.85009100
C 3.58519200 -0.43383000 -1.15203000
C 3.05791300 0.93851900 -0.79202300
H 3.19057000 -1.92397300 1.70976900
H 4.48425400 -0.32935700 -1.76976200
H 2.81956000 -0.98027900 -1.72317400
H 3.81922200 1.52395400 -0.25808000
H 2.69735400 1.48668800 -1.66876100
H 2.04693000 -1.89786100 0.33391800
N 1.86543200 0.79437800 0.11882600
O 3.95647500 -1.14463800 0.00456800
C 2.29479300 -0.01496700 1.32349600
H 1.40238600 -0.13379300 1.94430800
H 3.06188800 0.56508400 1.85501400
C 1.39707400 2.14093700 0.54137400
H 1.03649700 2.65223900 -0.35471300
H 0.57816000 2.00319400 1.25147400
H 2.22154900 2.68981400 1.01050400
O 0.90921000 0.13044900 -0.59054800

OsO₃

Os 0.00000000 0.00000000 0.00000000
O 0.00000000 1.69370800 0.00000000
O -1.46679400 -0.84685400 0.00000000
O 1.46679400 -0.84685400 0.00000000

OsO₃.NMO

Os -1.36747700 -0.09381800 -0.04210900
O -3.02645800 -0.10251800 -0.41989400
C 2.29756900 -1.17918200 1.11080200
C 3.24983700 -0.85096500 -0.97041900
C 2.96430200 0.63406600 -0.94260400
H 1.45478500 -1.73855600 0.67545600
H 4.16611600 -1.03559300 -1.54245400
H 2.41204400 -1.37640100 -1.45541000
H 3.79585700 1.18404300 -0.48104100
H 2.74478100 1.03743000 -1.93646800
H 2.51447400 -1.58964000 2.10327100
N 1.73475800 0.90294000 -0.11305400
O 3.46436000 -1.33268500 0.33304200

cartesian

coordinates

C 1.94089300 0.28570300 1.25034000
H 1.01535700 0.45566500 1.80970800
H 2.76446700 0.83972300 1.72130500
O -0.76587300 -1.70047800 -0.08631200
C 1.52712200 2.37382800 0.00128800
H 2.41452900 2.83401900 0.45027500
H 1.36111600 2.74705700 -1.01250000
H 0.63914200 2.54048400 0.61315700
O -1.03762900 1.22530600 1.02680000
O 0.69359700 0.32670600 -0.80990000

OsO₃.NMO-TS

Os -1.30271500 -0.10294800 -0.04682400
O -0.68161500 -1.37308600 0.95397200
O 0.42460800 0.31644500 -0.76163800
C 2.42541800 -1.33339000 0.84630000
C 3.16795700 -0.58677100 -1.21030100
C 2.80393300 0.85116800 -0.89771500
H 2.74297500 -1.90613100 1.72414500
H 4.03813100 -0.60597800 -1.87595300
H 2.32354900 -1.08157200 -1.71614900
H 3.67175200 1.38122200 -0.47235100
H 2.44728500 1.38718400 -1.78462400
H 1.56670500 -1.84905900 0.38653100
N 1.72169100 0.91057700 0.10582200
O 3.52252100 -1.27245800 -0.03631000
C 2.01006200 0.05797600 1.27854700
H 1.11398300 0.02950800 1.90979400
H 2.82863600 0.55083600 1.82879300
C 1.37200400 2.28568500 0.46812800
H 1.11809900 2.82760600 -0.44729200
H 2.22921300 2.75908800 0.96878700
H 0.49820900 2.27431400 1.12646400
O -2.70496000 -0.68780200 -0.84167800
O -1.59808900 1.52127600 0.46814900

OsO₃.NMO.H₂O

Os 1.32340000 -0.34119000 0.05617000
O 2.82895600 -1.08897900 0.26243700
C -2.43167900 -0.51185900 -1.49826700
C -3.32406100 -1.33248900 0.46891400
C -2.93640500 -0.09151000 1.23586000
H -1.61998300 -1.25029700 -1.47428700
H -4.23839700 -1.74833900 0.90070500
H -2.52534500 -2.08345300 0.54486400
H -3.74241700 0.64941000 1.19753300
H -2.67186400 -0.30881400 2.27322900
H -2.68385100 -0.31076300 -2.54201000
N -1.72094700 0.55076700 0.62388200
O -3.59242100 -1.01869800 -0.87388400
C -1.98471500 0.77390200 -0.84495000
H -1.07427000 1.18946200 -1.28487700
H -2.77521500 1.53130000 -0.89782500
O 0.62498300 -0.88907200 -1.40339800
C -1.45704600 1.84670700 1.30875200

H -2.36530100 2.45298900 1.27158700
H -1.17966700 1.61555400 2.33737700
H -0.64319300 2.35903400 0.80145500
O 1.43273900 1.26835400 0.67875600
O -0.68065700 -0.34932200 0.85236700
O 0.37397100 3.03389500 -1.18506800
H 0.83743200 3.57884600 -1.82253600
H 1.05313300 2.64219900 -0.61286600

OsO₃.NMO.H₂O-TS

Os -1.35628000 -0.21907200 -0.06475500
O -0.86775500 -1.57284600 0.91177300
C 2.64550600 -1.77263800 -0.13244600
C 3.26996500 0.17321800 -1.22665900
C 2.77625300 1.04662200 -0.09022200
H 1.82832600 -1.96318200 -0.84785200
H 4.13077500 0.65375900 -1.70456300
H 2.47734800 0.04778000 -1.98127900
H 3.59649400 1.22998300 0.62389600
H 2.37463600 2.00883100 -0.42830700
H 3.04341800 -2.73670200 0.20230200
N 1.70801300 0.35961600 0.66714800
O 3.70427300 -1.07616300 -0.74628900
C 2.11811900 -1.00723700 1.06261500
H 1.25170200 -1.49929000 1.51708600
H 2.91714500 -0.88475600 1.81390400
O -1.76008800 1.35081800 0.51731100
C 1.21277100 1.16219600 1.78573300
H 2.03389200 1.31743600 2.50092700
H 0.86150200 2.11926300 1.38606700
H 0.39869600 0.62432600 2.28286800
O -2.59010900 -0.77711100 -1.11529200
O 0.45953200 0.20801900 -0.47925100
O 0.35112000 3.12100100 -0.62942500
H 0.20568600 2.20308800 -0.91310700
H -0.50989700 3.36889200 -0.26530700

OsO₃.2NMO-TS

Os 0.06116700 -0.42476800 -0.45539100
O -0.16227000 -2.06131800 -0.92989000
O 1.91818700 -0.45235300 -0.65782700
O -2.11200100 -0.39853100 -0.59367400
C 4.48546300 0.82645800 -0.86731100
C 3.07775200 2.07130000 0.47965100
C 2.79064700 0.89677200 1.38442000
H 5.49962800 0.80602400 -1.27487200
H 3.03986300 2.99385800 1.06388700
H 2.32351100 2.13261800 -0.31835600
H 3.52105700 0.87398600 2.20972500
H 1.77104700 0.90705300 1.77552600
H 3.77147900 0.86470400 -1.70111200
N 2.95336600 -0.37880400 0.64859100
O 4.37617300 1.97803600 -0.06815600
C 4.25241400 -0.42517400 -0.04729900
H 4.25405700 -1.32118100 -0.67436200
H 5.02758100 -0.52080400 0.72718300
C 2.73362500 -1.57394700 1.46577700
H 3.59650400 -1.71504700 2.13039300
H 2.63715900 -2.44294200 0.79265200
H 1.80430000 -1.44187900 2.01961200
O -0.12695300 1.14159900 -1.14708700
C -3.09464900 2.04388400 0.52264600
C -4.61127500 0.86129700 -0.77222000

C -4.33353800 -0.42162400 -0.02372800
H -3.01317700 2.93916900 1.14389000
H -5.65309000 0.86573300 -1.10395300
H -3.95747800 0.91996200 -1.65293800
H -5.00633300 -0.52566400 0.83475900
H -4.40569800 -1.29816600 -0.67194000
H -2.39358500 2.13140500 -0.31920200
N -2.92943600 -0.41393200 0.50982600
O -4.43047800 1.97808800 0.06312300
C -2.74760900 0.83112100 1.34791900
H -1.70166200 0.81151400 1.67172800
H -3.42170400 0.73393100 2.20735900
C -2.69227500 -1.63519800 1.32771100
H -2.76644200 -2.48847600 0.65208400
H -3.44268300 -1.68812800 2.12099500
H -1.68204500 -1.55329000 1.73552000
O 0.06461100 -0.31248100 1.36186100

NMO

O -0.93819900 0.00010400 1.41205000
C 1.29709600 1.16038100 0.13140900
C 1.29755400 -1.16022600 0.13136300
C -0.11117400 -1.22059500 -0.40950600
H 1.87651400 2.02049200 -0.22280100
H 1.87722600 -2.02015400 -0.22290500
H 1.24873800 -1.17987200 1.23109700
H -0.11552800 -1.23512900 -1.50925600
H -0.66545100 -2.07668400 -0.00985000
H 1.24821900 1.17999000 1.23116100
N -0.86207500 -0.00010600 0.07746700
O 1.95775400 0.00021300 -0.32467300
C -0.11150000 1.22044200 -0.40977500
H -0.66605200 2.07645200 -0.01031600
H -0.11578900 1.23470100 -1.50952000
C -2.22923000 -0.00017300 -0.50589700
H -2.20353700 -0.00005900 -1.60371200
H -2.73143400 0.89092000 -0.12026200
H -2.73129800 -0.89142700 -0.12048200

NMM

C -1.18388100 1.15716200 -0.19409600
C -1.18402900 -1.15713100 -0.19400000
C 0.28531100 -1.18757500 0.17369400
H -1.71368700 2.01666900 0.23346000
H -1.71379000 -2.01656500 0.23378700
H -1.28397200 -1.19274800 -1.29544200
H 0.38223600 -1.25327500 1.28095500
H 0.76486900 -2.07957300 -0.25625600
H -1.28359100 1.19265000 -1.29557200
N 0.94792400 -0.00001300 -0.33876400
O -1.80926100 0.00007600 0.31004000
C 0.28540900 1.18756900 0.17380900
H 0.76506600 2.07954700 -0.25606100
H 0.38224600 1.25312600 1.28107200
C 2.35260200 -0.00005700 -0.00458600
H 2.53112600 -0.00080200 1.09204100
H 2.83767300 0.88964300 -0.42731500
H 2.83797100 -0.88899600 -0.42856100

NMM-H⁺

C 0.12117000 -1.23253200 1.15810800
C 0.12117000 -1.23253200 -1.15810800
C 0.12117000 0.28161000 -1.23835700
H 0.65568400 -1.64432100 2.01996000
H 0.65568400 -1.64432100 -2.01996000
H -0.91557600 -1.61937300 -1.18944900
H 1.14401400 0.67781000 -1.24766300
H -0.42526100 0.66185700 -2.10893200
H -0.91557600 -1.61937300 1.18944900
N -0.53438000 0.84813400 0.00000000
O 0.77896400 -1.66581400 0.00000000
C 0.12117000 0.28161000 1.23835700
H -0.42526100 0.66185700 2.10893200
H 1.14401400 0.67781000 1.24766300
C -0.53548800 2.34028300 0.00000000
H -1.04739700 2.69827400 -0.89737800
H -1.04739700 2.69827400 0.89737800
H 0.50328600 2.68306800 0.00000000
H -1.51241700 0.52738300 0.00000000

H₂O

O 0.00000000 0.11835700 0.00000000
H 0.76090900 -0.47336600 0.00000000
H -0.76090900 -0.47348800 0.00000000

(E)-2-Butene (8)

C 0.54630300 1.87342300 0.00009100
H 1.06468300 2.27887200 0.88091300
H 1.06470500 2.27907800 -0.88061400
H -0.47693200 2.27066300 0.00012400
C 0.54630300 0.38158600 -0.00015800
H 1.52499500 -0.10935900 -0.00001700
C -0.54630300 -0.38158600 -0.00015800
H -1.52499500 0.10935900 -0.00001700
C -0.54630300 -1.87342300 0.00009100
H -1.06468300 -2.27887200 0.88091300
H -1.06470500 -2.27907800 -0.88061400
H 0.47693200 -2.27066300 0.00012400

9

C -0.67211500 0.35692900 0.38421700
H -0.71851600 0.91785900 1.34090100
C 0.67212000 -0.35696700 0.38417400
H 0.71853100 -0.91799200 1.34080300
C 1.83130500 0.61780800 0.31837100
H 2.79261100 0.08736500 0.37583400
H 1.78829900 1.17630500 -0.62304100
H 1.79673600 1.33383300 1.14994600
C -1.83130000 -0.61784200 0.31833200
H -1.79671600 -1.33395300 1.14983200
H -2.79260700 -0.08740800 0.37586300
H -1.78830500 -1.17624000 -0.62314000
O 0.68946400 -1.25492500 -0.70597300
H 1.59396100 -1.57568800 -0.81162000
O -0.68947500 1.25499400 -0.70584300
H -1.59396300 1.57580600 -0.81141400

10

Os 0.78795500 0.00000000 0.00000000
O 1.68571300 -1.24748200 0.74328400
O -0.41447100 0.65445000 1.09323400
O -0.41447100 -0.65445000 -1.09323400
O 1.68571400 1.24748200 -0.74328400
C -2.40729800 -0.52697500 -0.44864100
C -2.40729800 0.52697500 0.44864100
H -2.59986700 -0.29966400 -1.49757700
H -2.59986700 0.29966300 1.49757700
C -2.54931700 -1.94395600 -0.01026500
H -3.60748300 -2.24226500 0.01878100
H -2.03293700 -2.62535300 -0.69560200
H -2.13223300 -2.08501400 0.99615000
C -2.54931800 1.94395600 0.01026500
H -2.03294000 2.62535300 0.69560300
H -2.13223200 2.08501500 -0.99614900
H -3.60748500 2.24226300 -0.01878200

11

C -0.27836800 0.70270900 -2.00097900
C 0.27836800 -0.70270900 -2.00097900
H -0.27200800 -1.35203700 -2.69918600
H 0.27200800 1.35203700 -2.69918600
Os 0.00000000 0.00000000 0.74335700
O 0.00000000 1.23895700 -0.69164400
O 0.00000000 -1.23895700 -0.69164400
O 1.48345300 -0.05820700 1.56704700
O -1.48345300 0.05820700 1.56704700
C 1.76686100 -0.77093600 -2.26133700
H 2.13909800 -1.78594200 -2.08472700
H 1.99314800 -0.49093700 -3.29810600
H 2.30806100 -0.08439700 -1.59486600
C -1.76686100 0.77093600 -2.26133700
H -2.13909800 1.78594200 -2.08472700
H -1.99314800 0.49093700 -3.29810600
H -2.30806100 0.08439700 -1.59486600

11_{H2O}

O 0.78322600 0.84676300 -0.93462900
O 0.78054500 -0.57869200 1.11634200
C 2.10224800 0.64461400 -0.42127000
C 2.06969000 -0.57778300 0.49180700
H 2.74827200 0.44866500 -1.29287100
C 2.29332400 -1.88601700 -0.23535500
H 2.80255300 -0.46220000 1.30591200
H 2.12014900 -2.73297100 0.43829900
H 1.61065600 -1.98278100 -1.09151900
H 3.32174400 -1.94655300 -0.61412900
Os -0.63301300 -0.07340800 -0.06580100
C 2.53261300 1.91008400 0.28750500
H 3.58658700 1.85371800 0.58902400
H 2.40021300 2.77645100 -0.36928100
H 1.92163500 2.06445000 1.18783400
O -1.62384700 1.47297200 -0.55233200
H -2.33346300 1.57675600 0.11071300
O -1.63334300 0.12258000 1.54336100
H -1.16293100 -0.34833000 2.25565400
O -1.16828700 -1.39032200 -0.95459700

11_{H₂O,NMM}

C -2.91239300 0.67564100 0.20072400
O -2.28239900 -0.53050000 -0.25919500
Os -0.39851400 -0.53249200 -0.21115300
O -0.63450400 1.29430200 0.40327100
C -1.91048300 1.81579700 0.04915300
C -1.87988400 2.39773400 -1.35201600
O 0.12855400 -0.27682700 -1.80502200
H -3.77978400 0.83172000 -0.46106200
H -2.14191200 2.61068200 0.77768700
H -1.06832600 3.13043600 -1.44077800
H -1.72008600 1.61452600 -2.10511300
H -2.82711600 2.90413200 -1.58094100
C 2.46178800 1.79184000 -0.75619900
C 2.32360200 1.43267700 1.52452100
C 2.54097000 -0.05423200 1.34541900
H 2.99596200 2.38612300 -1.50725900
H 2.77128100 1.75161900 2.47318700
H 1.24554700 1.65582500 1.54814500
H 3.62137100 -0.27991200 1.40216100
H 2.00616400 -0.61115800 2.11983400
H 1.38474800 2.02266600 -0.82930200
N 2.05355200 -0.52026200 0.02227300
O 2.96513200 2.16886300 0.50304400
C 2.70483500 0.31951400 -1.01443900
H 2.32734800 0.01980900 -1.99750000
H 3.79153800 0.12399100 -0.97479700
C 2.47971800 -1.90856600 -0.16980000
H 2.09605300 -2.52440500 0.65460400
H 3.57916000 -1.98724200 -0.16044600
H 2.10571700 -2.28437600 -1.13014700
C -3.36237300 0.46180000 1.63066100
H -3.94896900 1.32050000 1.98263500
H -3.98393000 -0.43793300 1.70237700
H -2.48921400 0.33882100 2.28387300
O -0.61289700 -2.47622600 -0.24479200
H 0.19409800 -2.93055200 0.04204800
O -0.13729700 -0.84856300 1.71222300
H -0.33488000 -1.78566000 1.86815100

11_{NMM}

C -3.02673900 -0.65939500 0.08769900
O -2.05901700 -0.69098900 -0.96244100
Os -0.31731400 -0.09858500 -0.39296000
O -1.26100700 0.56068700 1.13107500
C -2.69497300 0.52365200 0.98342000
C -3.16527600 1.84785800 0.42122800
O 0.38358800 -1.64665400 -0.14757400
O -0.10624100 1.10673100 -1.60641100
H -4.00269000 -0.50047700 -0.40040600
H -3.09335400 0.36943500 1.99940300
H -2.78207000 2.67912800 1.02506000
H -2.80700300 1.97243600 -0.61009800
H -4.26173300 1.90153100 0.41265400
C 2.98442600 -1.15082700 1.24916400
C 3.39937600 -0.41045700 -0.89775700
C 2.74005900 0.92649700 -0.64187900
H 3.49298700 -1.51332400 2.15063600
H 4.20668000 -0.28766800 -1.62891900
H 2.67342400 -1.13711000 -1.30327200

H 3.50843400 1.63641100 -0.28781400
H 2.27126200 1.33409800 -1.54650200
H 2.29717100 -1.93330500 0.89698400
N 1.68807300 0.82503400 0.39930200
O 3.98294100 -0.90223400 0.28626000
C 2.22857800 0.12010700 1.59344400
H 1.38901100 -0.08615500 2.27186800
H 2.92141400 0.81410100 2.10091900
C 1.30396600 2.18977400 0.81133900
H 2.17647800 2.71654800 1.22773900
H 0.51043600 2.12846500 1.56314500
H 0.92949300 2.73594700 -0.06009700
C -3.03043300 -1.98240100 0.82814000
H -3.85907100 -2.02544300 1.54774700
H -3.13842000 -2.81053200 0.11876000
H -2.08911700 -2.12605600 1.37597200

11_{2NMM}

C -0.17297700 3.07041700 -0.07260500
O 0.73250700 1.96493900 -0.07244900
Os -0.16717700 0.25804400 -0.14270500
O -1.72944700 1.29328900 0.26083200
C -1.42126600 2.63717200 0.67677900
C -1.26013100 2.66956900 2.18200400
O -0.20373300 0.02433500 -1.85418200
O 0.33239600 -0.40629900 1.37474000
H 0.33231500 3.88303800 0.47643600
H -2.28876000 3.24459600 0.37060300
H -2.13800600 2.22649600 2.66832000
H -0.37260900 2.09872600 2.48649200
H -1.14944800 3.70144800 2.54075000
C -3.08875300 -1.39995400 1.43981100
C -3.59731900 -1.02919000 -0.78789000
C -2.40520700 -1.84439100 -1.24388100
H -3.52663200 -1.77265500 2.37330800
H -4.41063300 -1.13872500 -1.51509000
H -3.32956000 0.03689000 -0.71718800
H -2.71962900 -2.89226900 -1.39956900
H -1.99264200 -1.45373700 -2.18223400
H -2.78950200 -0.34816100 1.58703400
N -1.32088700 -1.83906900 -0.23351700
O -4.08798400 -1.49735100 0.44949400
C -1.88511800 -2.24243100 1.07561100
H -1.09239000 -2.14754000 1.82725100
H -2.19143600 -3.30168800 1.00405200
C -0.30364100 -2.81713600 -0.63089900
H -0.74624200 -3.82241800 -0.72710100
H 0.48283000 -2.84547200 0.13214800
H 0.12497800 -2.51778600 -1.59476200
C -0.45317700 3.50549500 -1.49763900
H -1.03846600 4.43464800 -1.51706500
H 0.48977900 3.67654400 -2.03079500
H -1.01228800 2.72975700 -2.03717400
C 3.48407000 0.24464700 1.42418000
C 3.16954600 -2.01393500 1.02934300
C 3.08199000 -1.77179100 -0.46585400
C 3.39458700 0.55053800 -0.05547000
H 3.62027700 -2.99512500 1.22475400
H 2.49092000 0.35087000 1.89263100
H 4.17819400 0.94146100 1.90918300
H 4.09868900 -1.87170300 -0.90072400
H 2.44279700 -2.52376200 -0.95061800

H 4.41607400 0.52617800 -0.48888300
H 2.96293400 1.54472900 -0.21597900
H 2.16072600 -1.98903400 1.47936900
C 2.60876100 -0.18058800 -2.18585500
H 2.22693400 0.82617300 -2.39333000
H 3.64515700 -0.26145300 -2.56625800
H 1.97366900 -0.89685100 -2.72012900
O 3.99566300 -1.05456400 1.64406000
N 2.55431900 -0.43520000 -0.75442900

11_{NMO}

C -3.07831700 0.57640800 0.57953100
O -2.59422000 -0.55067600 -0.14671400
Os -0.67638500 -0.58271600 -0.31673200
O -0.81312900 1.23683800 0.26188500
C -2.16082800 1.74698700 0.26906400
C -2.45678000 2.40010700 -1.06357000
O 1.52458600 -0.58804200 -0.67152700
O -0.36943000 -1.66594900 0.98953600
O -0.61035800 -0.70354500 -2.02346400
H -4.09196400 0.77864300 0.19468200
H -2.19059200 2.49347100 1.08008200
H -1.68240900 3.13535600 -1.31114400
H -2.48648100 1.64551600 -1.86121700
H -3.42806100 2.91154000 -1.03826300
C 3.70127600 1.23233800 -0.82587500
C 2.18204100 1.83829900 0.80479200
C 2.16002300 0.44925700 1.40230600
H 4.67104300 1.50950200 -1.25473700
H 2.01353300 2.57439700 1.59861500
H 1.37651500 1.94011100 0.06279300
H 2.94123300 0.34140200 2.16696300
H 1.18664600 0.18802300 1.82866500
H 2.92958500 1.31921900 -1.60648500
N 2.46350800 -0.57465400 0.33209000
O 3.44458600 2.11420900 0.23894800
C 3.76408700 -0.19394800 -0.32800400
H 3.90164500 -0.91450100 -1.14063400
H 4.55709800 -0.30952100 0.42339200
C 2.60116500 -1.93395500 0.92864800
H 3.40531700 -1.92577300 1.67320700
H 2.83426300 -2.61496500 0.10602000
H 1.63970400 -2.20314000 1.37080800
C -3.14484600 0.25175800 2.05957900
H -3.64296300 1.05754000 2.61584100
H -3.70025100 -0.67970500 2.21619700
H -2.13632500 0.11566300 2.47407300

11_{2NMO}

C -0.05845100 2.62675200 -0.87687800
O -0.06049700 1.38403600 -1.49178200
Os 0.09397200 -0.20593500 -0.27320600
O -0.52648800 1.29282400 0.99762500
C -0.90018000 2.48148400 0.39447800
C -0.73586700 3.63628300 1.36403600
O -1.90683400 -0.49969000 -0.69959100
O 2.04830600 0.45898800 -0.02398300
H 0.97223500 2.89436100 -0.54850600
H -1.96694500 2.43075500 0.06304400
H -1.31597200 3.45484700 2.27754500
H 0.32193700 3.73401000 1.65049500

H -1.06830200 4.58810900 0.92679100
C -3.62494700 -0.01750900 1.54274100
C -4.66065100 -0.17248600 -0.52446600
C -3.96341400 -1.47856200 -0.84447900
H -3.85031000 0.09960400 2.60846500
H -5.64845500 -0.16831500 -1.00006800
H -4.07183500 0.66808900 -0.92385600
H -4.55406400 -2.33317300 -0.48845100
H -3.74242700 -1.58358300 -1.91185300
H -2.99786500 0.82987100 1.22430800
N -2.63580000 -1.53522100 -0.13944200
O -4.86198600 -0.04238300 0.85938700
C -2.86376700 -1.30519000 1.34075000
H -1.86633700 -1.27648200 1.79588400
H -3.43828200 -2.17174900 1.69711300
C -1.98145500 -2.84906800 -0.38200000
H -2.67066300 -3.64798700 -0.08724400
H -1.06669800 -2.87301200 0.21620000
H -1.73904100 -2.89624400 -1.44714700
C -0.57800400 3.67576000 -1.83867600
H -0.54772000 4.68008500 -1.39387300
H 0.02413100 3.68491700 -2.75483600
H -1.61547100 3.44524800 -2.11872900
O 0.58169000 -1.19602800 -1.62807900
C 3.63496700 -1.89672600 -0.46600900
C 4.76103500 0.11977400 -0.63419200
C 4.21197000 0.60516700 0.69159400
H 3.80142800 -2.97896300 -0.50564800
H 5.76066200 0.54402400 -0.78517700
H 4.10558000 0.45681500 -1.45172200
H 4.87687700 0.32578200 1.51960900
H 4.03119900 1.68527300 0.69680100
H 2.93615600 -1.61800700 -1.27246000
N 2.87934300 -0.03460600 0.96481900
O 4.89474200 -1.27931800 -0.63619700
C 3.04374200 -1.53493500 0.87711000
H 2.04672000 -1.95866500 1.04496100
H 3.72184800 -1.81640300 1.69439500
C 2.37437800 0.38235200 2.30433800
H 2.22701000 1.46472200 2.25938500
H 3.11089400 0.10120000 3.06530000
H 1.41046500 -0.11246200 2.45608800
O 0.08237500 -1.19985100 1.22126200

11_{NMO, NMM}

C 3.36272000 -0.66563500 0.62579700
O 2.60264000 0.49067500 0.28254900
Os 0.73646900 0.08585200 -0.05341900
O 1.35743000 -1.76351300 -0.05889500
C 2.78439800 -1.85658300 -0.12643900
C 3.22998800 -1.91414200 -1.57457700
O 0.17475200 0.18647800 1.59122000
O 0.72378300 0.37690000 -1.76764600
H 4.39288300 -0.47214400 0.27842600
H 3.05679200 -2.79518900 0.38714600
H 2.70300600 -2.71817400 -2.10510800
H 3.01178600 -0.96547200 -2.08127800
H 4.30908300 -2.10757900 -1.64370400
C -2.36224900 -2.07314300 1.68271600
C -3.99684900 -1.18655500 0.28079000
C -3.26315600 -1.65778600 -0.95636000

H -2.24903200 -2.75617800 2.53183600
H -5.07648100 -1.21945900 0.09311200
H -3.71389600 -0.14461100 0.50371400
H -3.58053500 -2.67127500 -1.23630500
H -3.39145000 -0.97237400 -1.80163200
H -1.98891100 -1.08068700 1.97969500
N -1.78420500 -1.71049200 -0.68704300
O -3.73998000 -2.03857200 1.36848200
C -1.55349300 -2.59396700 0.51737300
H -0.47409100 -2.58308200 0.70488000
H -1.87750900 -3.60473300 0.23219200
C -1.07516500 -2.24964200 -1.88258500
H -1.50850000 -3.22104900 -2.14634600
H -0.01553900 -2.34253200 -1.62530800
H -1.20500600 -1.51831900 -2.68440700
C 3.36317600 -0.86740500 2.12965600
H 4.04913800 -1.67700500 2.41503200
H 3.68262900 0.05223000 2.63402900
H 2.35607100 -1.11859800 2.48590600
C -2.01727700 2.51544400 -1.20225200
C -2.00417400 2.44495600 1.11405600
C -0.55465400 2.87177100 1.16689600
C -0.55663900 2.91004100 -1.23672000
H -2.53495600 2.83621800 1.99033800
H -2.10864700 1.42196000 -1.29371400
H -2.53715000 2.98952500 -2.04416900
H -0.50079600 3.97421200 1.22693700
H -0.05795200 2.43802100 2.04196400
H -0.47723100 4.01198700 -1.27137800
H -0.06474900 2.48541500 -2.11978800
H -2.06197900 1.34480900 1.12658400
C 1.50163300 3.08830400 -0.03843600
H 2.05799900 2.78103300 -0.92975500
H 1.38549400 4.18465300 -0.03455800
H 2.06436700 2.76965900 0.84364600
O -2.65347500 2.96885400 -0.02485000
N 0.18074100 2.44041200 -0.04109800
O -1.40787800 -0.41450100 -0.42844600

11_[ox]

C 2.11209400 -0.62072700 -0.45180500
C 2.10009800 0.63014700 0.42715500
H 2.86088500 0.54125600 1.22029100
H 2.76989200 -0.47294100 -1.32422800
Os -0.70725900 -0.00587700 0.00854300
O 0.80059300 -0.72476300 -0.97705500
O 0.84359700 0.57865500 1.05067400
O -1.15984300 1.55174300 -0.51842600
O -1.43996700 -0.36876700 1.50576900
O -1.58288700 -1.03634000 -1.04683300
C 2.27845300 1.91799800 -0.34908000
H 1.58794500 1.96543400 -1.20185500
H 2.08551100 2.78220900 0.29587100
H 3.30357100 1.99145800 -0.73508600
C 2.47110700 -1.88558700 0.29433500
H 2.30532800 -2.76368000 -0.33896300
H 3.52446100 -1.86891500 0.60130700
H 1.85164500 -1.98336600 1.19674000

11_{[ox]NMM}

C 1.63811400 1.99057500 0.40814700
O 0.60823900 1.19089400 -0.11274900
Os 0.83626600 -0.76135800 -0.06773000

O 2.65639400 -0.08617600 0.02573800
C 2.91097500 1.30198300 -0.08462700
C 3.27587800 1.64920600 -1.51022800
O 0.17025300 -0.99475500 1.48371700
O -0.39115300 -0.80428700 -1.25211000
H 1.54474400 2.98666400 -0.05556800
H 3.74958500 1.50776700 0.60116200
H 4.09249800 1.01005400 -1.86273300
H 2.40898300 1.50402400 -2.16956200
H 3.59375200 2.69684500 -1.58556300
C 1.55091000 2.08847400 1.91739600
H 2.28957700 2.80611700 2.29772000
H 0.55277700 2.42322400 2.22375000
H 1.74491000 1.11626100 2.38985400
C -2.58803100 1.68658300 -0.89816000
C -3.79727000 -0.22386600 -1.39453100
C -3.88041900 -0.59299300 0.07288900
C -2.63097500 1.36709600 0.58256100
H -4.69354400 -0.55888900 -1.93056800
H -1.66232400 1.26767500 -1.33656800
H -2.59152500 2.77172700 -1.05908100
H -4.82662100 -0.18488300 0.49476900
H -3.90748100 -1.68659100 0.18935400
H -3.49815200 1.89213300 1.04366100
H -1.71379700 1.73102700 1.07051500
H -2.91224100 -0.70873600 -1.84558900
C -2.80174600 -0.38386300 2.19813800
H -3.70499600 0.04619200 2.68156000
H -2.82075800 -1.47275200 2.33742300
H -1.91292300 0.00769300 2.71094500
O -3.72122800 1.17347100 -1.56099500
N -2.72933800 -0.06854300 0.78992800
O 1.64650200 -2.24311300 -0.37448000

12

Os -0.69116500 -0.09877700 0.00210400
O 0.96148500 -0.75972900 1.06337000
O 0.62395800 0.76415100 -1.07625600
C 2.16922000 -0.52328300 0.31225700
C 1.96921600 0.71651700 -0.57258900
H 2.97255100 -0.33486100 1.03975600
C 2.23639600 2.01704700 0.15698500
H 2.62634500 0.63026400 -1.45267400
H 2.03294800 2.86823000 -0.50128500
H 1.58823300 2.11104500 1.03926700
H 3.28235000 2.07222200 0.48530500
O -1.39968500 -1.57796100 -0.40355700
O -1.91963800 1.18924200 -0.65902400
O -0.69713800 0.66955300 1.64271100
H 0.46733700 -0.01657400 1.79657800
C 2.45632200 -1.77409400 -0.48613300
H 3.42369000 -1.68788300 -0.99688600
H 2.48108700 -2.65095200 0.16928700
H 1.68139200 -1.93610900 -1.24814700
H -1.56614600 1.55251000 -1.49215200

12_{NMM}

C -2.97737800 0.86877300 0.32019300
O -1.65018600 1.18125100 0.76102800
Os -0.25077700 -0.24813000 -0.14556300

O -1.87553000 -0.95942000 -0.85275900
C -3.05261900 -0.60390000 -0.12006200
C -3.26937100 -1.55782600 1.03924200
O -0.15783100 -1.12167000 1.32110400
H -3.64605000 1.00068200 1.18726800
H -3.88212500 -0.71673600 -0.83811500
H -3.20797000 -2.59629800 0.69343100
H -2.52419200 -1.41208900 1.83007300
H -4.26508700 -1.39599600 1.47308100
C 3.34739000 -1.16043500 0.32070300
C 3.26070500 0.55859500 -1.22495400
C 2.52900500 1.46107300 -0.25468500
H 4.05074800 -1.83476900 0.82345100
H 3.90271800 1.16905300 -1.87090700
H 2.54336100 0.01255500 -1.85711100
H 3.26444300 2.06154400 0.30938200
H 1.84140900 2.13184100 -0.78174900
H 2.62879200 -1.76709900 -0.25327400
N 1.73469600 0.68286200 0.73058100
O 4.10532800 -0.34204500 -0.54014700
C 2.62718400 -0.32600700 1.35888800
H 2.01885100 -0.94924000 2.02519100
H 3.37391000 0.21766200 1.96389000
C 1.26177700 1.60095600 1.78118400
H 2.11890100 2.07203200 2.28767000
H 0.66501000 1.04445000 2.51096900
H 0.63938300 2.38201000 1.33349800
C -3.40775600 1.80739500 -0.79350800
H -4.47409000 1.67514400 -1.01778700
H -3.25006000 2.85252600 -0.49895000
H -2.83883900 1.61377600 -1.71282100
O -0.26379600 1.36385300 -1.02781900
O 0.71949600 -1.28137200 -1.42700300
H 0.06074900 -1.82642800 -1.89821800
H -1.03714400 1.72671700 -0.19748100

12_{NMM.H2O}

Os -0.29367500 -0.61557600 -0.18049900
O -2.17084100 -0.83595900 -0.49469200
O -0.88822100 1.44922100 0.09621100
C -2.99418700 0.29877000 -0.22320500
C -2.20268700 1.59444900 -0.44509700
H -3.81443000 0.25938100 -0.96028300
C -2.11639000 1.97418800 -1.90977300
H -2.69884800 2.40879900 0.11385800
H -1.44222300 2.82883300 -2.03744400
H -1.72951000 1.14044400 -2.50861100
H -3.10795000 2.24713800 -2.29500500
O 0.21476500 -0.12511000 -1.73579500
O -0.06322400 -2.51250400 -0.32935700
C -3.57416700 0.17289300 1.17335700
H -4.29995200 0.97436800 1.36669400
H -4.08333900 -0.79073200 1.28636000
H -2.78265600 0.21977200 1.93078900
O -0.37916800 -0.61947000 1.64792400
H -0.43233600 0.39788500 2.22334200
O -0.53575300 1.61419100 2.43782700
H -1.31560800 1.79067900 2.98144900
H -0.79775700 1.71023200 1.28520200
H -0.93020400 -2.87613000 -0.58430100
N 2.02391100 -0.52536100 0.32978400
C 2.36359400 0.53491400 1.31379100
C 2.88685300 -0.34294700 -0.86843900

C 2.34759400 -1.82944800 0.94052500
C 2.33776200 1.91354900 0.69388300
H 3.38684100 0.33779900 1.67923900
H 1.67484600 0.45541200 2.16103100
C 2.89931600 1.08883300 -1.37601200
H 2.54462200 -1.03586300 -1.64727000
H 3.91510000 -0.62227200 -0.57875200
H 1.70483400 -1.98201200 1.81306800
H 3.40464800 -1.84316200 1.24817700
H 2.15537400 -2.62852800 0.22055900
H 2.62813600 2.65655500 1.44567100
H 1.32596400 2.16643700 0.33190200
O 3.27213700 1.98941700 -0.35933700
H 3.64680300 1.17530200 -2.17410300
H 1.91587100 1.36147200 -1.78856400

12_{NMO}

C -3.13411000 0.68175900 0.15337300
O -2.47503900 -0.27322400 -0.72584700
Os -0.54744100 -0.46562100 -0.17372500
O -0.79094500 1.33913500 0.65290000
C -2.09655000 1.82045400 0.32396700
C -2.01665700 2.69300800 -0.91651800
O 1.44708100 -0.81984400 0.27293800
O -0.96807300 -1.33792900 1.26468800
O -0.03521100 -0.02260100 -1.77803600
H -3.98832300 1.06995600 -0.42191000
H -2.43473800 2.42955900 1.18207600
H -1.26738000 3.47943700 -0.76587600
H -1.71626300 2.09733300 -1.78784600
H -2.98076100 3.17290300 -1.13328100
C 4.17933200 -0.57937400 -0.32063800
C 2.94339600 1.19217900 -1.15637500
C 2.26711000 1.43912100 0.17254100
H 5.20747600 -0.94571500 -0.21870000
H 3.05644900 2.14580000 -1.68361200
H 2.32431100 0.52183800 -1.77352500
H 2.86021400 2.12616300 0.79184700
H 1.24139100 1.81559200 0.07820200
H 3.60268900 -1.30532500 -0.91446300
N 2.18400300 0.14509600 0.94983500
O 4.24099900 0.66805000 -0.96434100
C 3.56424600 -0.44206200 1.05677100
H 3.44091700 -1.40763700 1.55836000
H 4.15513500 0.24064600 1.68130600
C 1.61687400 0.37780000 2.30734300
H 2.30652800 1.01310400 2.87387200
H 1.49810000 -0.60242100 2.77637200
H 0.64324100 0.86366200 2.18789000
C -3.61930100 0.06749500 1.44545000
H -4.24336300 -0.81247400 1.24668900
H -2.78757100 -0.23864500 2.08727300
H -4.23318500 0.80349500 1.98128600
O -1.30041200 -2.30232600 -1.06204000
H -2.48235200 -1.35595200 -0.86899400
H -1.05827500 -2.25217100 -2.00026000

12_{H2O}

Os 0.71276000 -0.11331300 -0.06524900
O -0.47659100 -1.03433600 1.10299200
O -1.08498400 0.55229100 -0.88777500
C -1.86959000 -0.72291500 0.96127600

C -2.15029100 -0.31254200 -0.48438700
H -2.41427000 -1.65194600 1.19414100
C -2.23259500 -1.48874100 -1.43290900
H -3.08544900 0.26984600 -0.52260500
H -2.31501000 -1.13696000 -2.46699600
H -1.33625900 -2.11871000 -1.35947500
H -3.10737200 -2.10950200 -1.19998300
O 1.21792000 -0.93041900 -1.45640500
O 2.13520200 -0.56115700 1.12693700
C -2.22193400 0.36200500 1.95652600
H -3.30227000 0.55668300 1.96422700
H -1.91095200 0.07314800 2.96609600
H -1.69901600 1.29456500 1.69925700
O 0.98543200 1.61139500 0.37032200
H 0.16808100 2.46873800 -0.22575500
O -0.74434800 2.87428400 -0.73650900
H -1.25769800 3.36179200 -0.07593200
H -1.14967600 1.77041600 -0.86762000
H 1.82555700 -1.28960000 1.69403200

12_{NMO,H2O}

C -2.76544700 1.28982200 0.60013100
O -2.51684400 0.05618600 -0.11674300
Os -0.51834500 -0.29725800 -0.29139900
O -0.41154600 1.62269900 0.11595600
C -1.68022100 2.25972500 0.11981500
C -1.98469800 2.82339500 -1.25717200
O 1.56497700 -0.55890300 -0.62843600
O -0.35325800 -0.82863800 1.36505200
O -0.54635400 -0.25213700 -2.02207200
H -3.75184600 1.64322100 0.26004700
H -1.62366000 3.08655200 0.85129200
H -1.15152200 3.45306800 -1.58927800
H -2.10903600 2.01415600 -1.98783400
H -2.89965300 3.43185500 -1.24557600
C 4.03831600 0.72894200 -0.85506400
C 2.69293000 1.71410700 0.75118800
C 2.40632100 0.38988300 1.42050300
H 5.04155400 0.77894500 -1.29417800
H 2.69936000 2.50248100 1.51186900
H 1.90159400 1.94568400 0.02122900
H 3.17077000 0.15479600 2.17328300
H 1.40871100 0.34825800 1.86642700
H 3.29520600 0.91985200 -1.64470300
N 2.47152700 -0.72415900 0.39586500
O 3.97318900 1.70537100 0.15261000
C 3.81682600 -0.65340600 -0.27857200
H 3.80440800 -1.42919900 -1.05095200
H 4.57054600 -0.88668000 0.48503700
C 2.29973200 -2.06244900 1.03198200
H 3.09185600 -2.20773400 1.77514800
H 2.36237700 -2.80122200 0.22915500
H 1.30470400 -2.09111900 1.48269000
C -2.77542900 1.06042800 2.09560300
H -3.45330100 0.23831000 2.36032500
H -1.77497400 0.80672200 2.46282500
H -3.12215500 1.96801700 2.60676600
O -0.79696800 -2.40949400 -0.55817200
H -0.82553600 -2.51600900 -1.52077600
H -2.11642100 -2.47616100 0.00789000
H -2.95893900 -0.91633400 0.22545200

O -3.07784200 -2.21417300 0.41704800
H -3.74328900 -2.57676200 -0.18333500

13

Os 0.82166700 0.03333700 0.00462000
O -1.44462400 0.68439100 1.18041500
O -0.72193200 -0.35219200 -1.10384400
C -2.48412300 0.13240700 0.37132100
C -1.84735900 -0.94649400 -0.52418100
H -3.25059200 -0.32635500 1.01881900
C -1.55912600 -2.24250000 0.21711400
H -2.53536900 -1.15919400 -1.36050600
H -0.95847600 -2.91315500 -0.40858600
H -1.00714700 -2.07550000 1.15339300
H -2.49813700 -2.75160400 0.47072600
O 1.91721500 -1.01963600 -0.75251100
O 1.12909700 0.23430900 1.66980200
O 0.50903100 1.74296700 -0.78194800
H -1.32306800 0.16792600 1.99127300
H 1.33215100 2.25911100 -0.76264000
C -3.06177000 1.26986200 -0.43571900
H -3.87367000 0.91294600 -1.08190400
H -3.45428300 2.05020300 0.22529000
H -2.27409700 1.70366100 -1.06353400

13_{H2O}

Os 0.78388000 0.03519500 -0.07730400
O -1.28453400 0.09120700 -1.10064100
O -0.22161400 -0.87268900 1.26892100
C -2.05387700 -0.87726200 -0.35439900
C -1.64485700 -0.82554200 1.12192600
H -3.11587900 -0.59587200 -0.43627100
C -2.18107000 0.39603400 1.84019100
H -2.02000900 -1.74057900 1.60983700
H -1.80308900 0.42772000 2.86768800
H -1.85961700 1.31478200 1.33082000
H -3.27846800 0.38135700 1.87202100
O 1.22526900 -1.00870500 -1.35200300
O 2.30644500 -0.16404700 1.04264100
O 0.60588300 1.75402100 0.05760100
H -1.66858200 1.00558600 -1.02226700
C -1.82703900 -2.23269600 -0.98241100
H -2.48333100 -2.97785300 -0.51593300
H -2.04300700 -2.19336100 -2.05512900
H -0.78761200 -2.55829100 -0.85575800
H 2.01245000 -0.66457700 1.82680900
O -1.77909100 2.72622900 -0.87952800
H -2.26830400 3.17202900 -0.17673300
H -0.83724900 2.78289300 -0.61774400

13_{NMO}

C -4.08954000 0.95577300 -0.49579300
O -4.79734700 0.50653900 0.63849900
Os -0.31190700 -0.29797500 0.27423900
O -2.21781700 -0.18174700 0.36615800
C -2.96864100 -0.03320200 -0.82978400
C -3.48630800 -1.38899200 -1.26704100
O 1.80887000 -0.45009000 0.60975000
O -0.27153000 -1.78834500 -0.60113400
H -4.81298500 0.94814200 -1.32735600

H -2.33262000 0.40827900 -1.62134700
H -2.66031500 -2.10056600 -1.38234200
H -4.18311300 -1.77225200 -0.51247300
H -4.01964500 -1.30721500 -2.22388900
C 2.88340800 1.84658300 -0.82590600
C 4.25749000 0.98769100 0.82122300
C 4.09981800 -0.42690700 0.30776100
H 2.85290700 2.60233200 -1.61790600
H 5.25133400 1.10076000 1.26920600
H 3.49760500 1.18776600 1.59356800
H 4.87311100 -0.65935700 -0.43625200
H 4.11323400 -1.17007600 1.11181300
H 2.08892100 2.07230000 -0.09894900
N 2.76768500 -0.58693300 -0.37619900
O 4.16278600 1.90913000 -0.23338300
C 2.64507500 0.48216900 -1.43500500
H 1.64329100 0.39432600 -1.86706600
H 3.40415800 0.25247500 -2.19458500
C 2.67872900 -1.94370900 -0.98476100
H 3.47764700 -2.05992800 -1.72487100
H 1.68634500 -2.05128600 -1.42995900
H 2.78637400 -2.66687100 -0.17208300
C -3.55214000 2.36110200 -0.29120000
H -4.36398600 3.03577700 0.00421600
H -2.79015400 2.36315400 0.50013400
H -3.08349000 2.74943300 -1.20609600
O -0.08686000 1.31966500 -0.28517000
H -4.11399700 0.29085900 1.29500400
O -0.38751500 -0.48142000 2.17216600
H 0.52446600 -0.57634900 2.50044900

13_{NMO.H2O}

C 4.12187100 -0.78694500 0.32291000
O 4.95516500 0.16612400 -0.27645800
Os 0.18956400 0.06673200 0.02182400
O 2.04330300 0.15441500 -0.42626300
C 2.83534200 -1.02583200 -0.48032200
C 3.10488700 -1.36077500 -1.93196300
O -1.88716000 0.39795900 0.45756100
O -0.29171800 -0.81690300 -1.38760800
H 4.67866500 -1.74006200 0.28362200
H 2.28484900 -1.85445000 0.00654000
H 2.16339100 -1.48969200 -2.47882000
H 3.68201600 -0.54891800 -2.38830700
H 3.69122000 -2.28629900 -2.01023600
C -4.61461400 1.10915100 0.40734900
C -3.88876100 0.14992900 -1.57580100
C -3.26300300 -1.02465200 -0.86350500
H -5.51650300 1.48409600 0.90406400
H -4.25370000 -0.17399000 -2.55612600
H -3.13225200 0.93717400 -1.72903000
H -3.98852600 -1.83925100 -0.73418300
H -2.35771700 -1.37853000 -1.36720100
H -3.89347000 1.93685400 0.32157600
N -2.83525000 -0.60488800 0.52537700
O -4.99963400 0.64236600 -0.86030000
C -4.02007000 -0.01014600 1.23676800
H -3.64623800 0.33783400 2.20550300
H -4.75306500 -0.81546100 1.37782600
C -2.32872800 -1.77954900 1.28506100
H -1.54279200 -2.25864400 0.69589300

H -3.15523000 -2.47841400 1.45169000
H -1.90948300 -1.41171800 2.22445700
C 3.82041400 -0.44647500 1.77313800
H 4.75684300 -0.32501700 2.33020800
H 3.25756300 0.49531600 1.83007400
H 3.21217100 -1.22176800 2.25814700
O 0.41023300 -0.46239900 1.64425200
H 4.55612200 1.05318200 -0.14181000
O 0.27375700 1.96709100 -0.18510900
H -0.61125600 2.33639000 -0.02042300
O 3.43330300 2.54062600 -0.10683000
H 3.07115300 2.79009700 0.75283100
H 2.74412000 1.95139000 -0.46834100

13_{NMM}

C 3.25373800 1.25843600 -0.03576900
Os 0.25344400 -0.76024900 -0.23480100
O 0.96394600 0.81111700 0.58607400
C 2.28223700 0.88839000 1.09159900
C 2.70441600 -0.33756200 1.88190400
O -0.31026600 -1.75566000 1.03792100
H 4.24863800 1.40061000 0.43418900
H 2.25466300 1.74846800 1.78673100
H 1.96236500 -0.57153700 2.65538600
H 2.81106100 -1.23259600 1.25309400
H 3.66784200 -0.14994400 2.37413900
C -2.96972000 1.67997100 -0.94567300
C -3.62741000 -0.45977200 -0.41004800
C -2.94224900 -0.40510600 0.93535000
H -3.37000400 2.66632600 -1.20880400
H -4.50773500 -1.11113500 -0.35934300
H -2.94083600 -0.87251500 -1.17617200
H -3.67331400 -0.03131700 1.67758100
H -2.60042400 -1.39748600 1.25634300
H -2.33566600 1.33411200 -1.77402000
N -1.77657200 0.49555700 0.91117100
O -4.07409500 0.81859900 -0.78659600
C -2.14718600 1.79830700 0.32443900
H -1.22074100 2.35289000 0.12615500
H -2.74016900 2.35632500 1.07423400
C -1.33810100 0.72033500 2.29251700
H -1.02815200 -0.23218500 2.73546200
H -2.16097200 1.14522600 2.89332000
H -0.49385200 1.41618700 2.29893700
C 2.83329800 2.52844100 -0.74041800
H 2.77335500 3.36669100 -0.03430100
H 3.55572500 2.77958400 -1.52472800
H 1.84952000 2.38025300 -1.20212600
O 1.03708400 -1.77053400 -1.36233400
O -0.19961800 0.56202000 -1.59874100
H -0.63779600 0.13075400 -2.34827400
O 3.30920400 0.25518600 -1.02508000
H 3.65657000 -0.56316600 -0.64450200

13_{NMM.H2O}

C -3.95038400 -1.34751600 -0.48397200
O -4.97601100 -0.52934000 0.00714100
Os -0.25337600 0.30571900 0.07811300
O -2.13270700 0.02232500 0.26382100
C -2.68491100 -1.28193600 0.38452800
C -2.97025500 -1.56920100 1.84386400
O 1.74098900 1.05548500 -0.16986100
O 0.18340600 -0.18356200 1.68193700

H -4.32105400 -2.38397700 -0.39036400
H -1.96298600 -2.01866400 -0.01992300
H -2.05964300 -1.47918500 2.44773400
H -3.71866600 -0.85704100 2.20919500
H -3.37485700 -2.58356500 1.96226200
C 5.23699800 0.05103700 -0.59085300
C 4.04869600 -1.85615800 -0.03648300
C 2.71818900 -1.13058700 -0.09793300
H 5.96868100 0.43152000 -1.31234700
H 3.89314500 -2.89343000 -0.35251700
H 4.44613400 -1.88326600 0.99463600
H 2.27737800 -1.18172500 -1.09963400
H 1.99832900 -1.51987300 0.63048500
H 5.68947200 0.13849100 0.41466900
N 2.87363700 0.34382300 0.18350800
O 4.99238600 -1.29268600 -0.91196500
C 3.96869100 0.87186400 -0.69943300
H 4.10724300 1.92399900 -0.42872600
H 3.55111900 0.81626800 -1.71020700
C 3.14112100 0.61112400 1.62727500
H 2.25448000 0.28257400 2.17652900
H 3.26667700 1.69167000 1.73086300
H 4.03899000 0.08302600 1.96239100
C -3.64736000 -1.05867900 -1.94474700
H -4.56179600 -1.15833700 -2.54140900
H -3.27389400 -0.03165000 -2.05580500
H -2.88438900 -1.73807700 -2.34772100
O -0.08815000 -0.54087500 -1.41097400
H -4.75178200 0.40287700 -0.20327600
O -0.78036600 2.13406900 -0.12423300
H 0.01978300 2.67296600 -0.25365000
O -3.92662500 2.07176100 -0.32994800
H -3.57755400 2.35594200 -1.18408800
H -3.15174700 1.65098200 0.08892400

13_{NMM.H2O(eq)}

C 3.71801200 -0.26294800 0.82099800
Os -0.01765700 0.43352000 -0.26594200
O 1.88356300 0.65581100 -0.39379100
C 2.79468200 0.95350900 0.65785300
C 2.13163500 1.34237100 1.96216800
O -0.46658000 2.09127700 -0.15612000
H 4.43900100 0.00232300 1.61434900
H 3.40422300 1.80090500 0.29226300
H 1.42369500 2.16872800 1.81979000
H 1.61660700 0.48136100 2.40421700
H 2.89769200 1.67644100 2.67454500
C -2.81735200 -1.96550700 0.75999900
C -3.10565300 0.06160300 1.82818500
C -3.11189800 0.82996100 0.52525600
H -3.28844800 -2.94725800 0.63105800
H -3.74713500 0.57111900 2.55642500
H -2.08574400 0.00324600 2.24733300
H -4.15332800 0.90598300 0.16634000
H -2.70234600 1.84132200 0.64073300
H -1.82015900 -2.11296600 1.19810800
N -2.31387000 0.14043600 -0.51999900
O -3.63845200 -1.22758700 1.63619700
C -2.72255500 -1.29079700 -0.59722000
H -2.01043900 -1.81261100 -1.25152100
H -3.71689900 -1.32109400 -1.07552000
C -2.60838200 0.77000400 -1.82349600
H -2.33975900 1.83012600 -1.77954400

H -3.68044100 0.67310700 -2.05325100
H -2.01531800 0.28166200 -2.60342600
C 4.48457500 -0.57671800 -0.45302500
H 5.05880100 0.28853800 -0.81089300
H 5.17649100 -1.40880100 -0.27709100
H 3.78465400 -0.87276200 -1.24591800
O -0.06334600 -0.85286900 0.86676200
O 0.28579400 -0.22216200 -2.05541200
H 1.23687300 -0.03461700 -2.20861200
O 3.02073900 -1.38372900 1.29233400
H 2.48867100 -1.75151900 0.55829100
O 1.67956200 -2.61349700 -1.01138800
H 2.31176000 -2.91981000 -1.67281100
H 1.07196400 -2.02080600 -1.48623800

14

Os -1.05664300 0.01306800 -0.02582800
O 3.16977700 -0.39192500 1.05880400
O 0.81044600 0.75468300 0.22751700
C 2.78485100 -0.54715100 -0.29154300
C 1.97656500 0.69492400 -0.63937800
H 3.67287900 -0.52222800 -0.95387500
C 2.74357700 1.98324400 -0.46481600
H 1.58677400 0.60112500 -1.66236400
H 2.11314200 2.84373300 -0.71194200
H 3.09281000 2.07961100 0.56864600
H 3.61868000 1.98911500 -1.12701200
O -2.28479600 1.18305700 0.00066000
O -1.33630700 -1.42782200 -0.88307300
O -0.46074400 -0.38757700 1.64562600
H 3.43500600 -1.25326500 1.40774800
H 0.82186500 0.28811800 1.19826900
C 2.03454500 -1.84640200 -0.51352000
H 1.61927700 -1.91302800 -1.52738400
H 2.70779600 -2.70318800 -0.37648700
H 1.21237100 -1.95416000 0.20661300

14_{NMO}

C 3.85794700 1.03789200 0.01328500
O 3.80275500 1.23825100 -1.38320000
Os 0.29485800 -0.28988000 0.01971400
O 2.26954300 -0.81682800 -0.37745300
C 3.43030800 -0.40423000 0.37368400
C 4.52363600 -1.39527500 0.03936700
O -1.56812800 0.54006900 0.01386700
O -0.34633300 -1.83379900 -0.45432300
H 4.92828100 1.09302800 0.27316300
H 3.15921500 -0.45614300 1.43843600
H 5.41109100 -1.21739700 0.66057300
H 4.17929600 -2.42239100 0.20189900
H 4.80801400 -1.28161800 -1.01468500
C -4.11684800 1.58165900 -0.42500700
C -3.80318200 -0.49475200 -1.40419600
C -3.27473300 -1.10376400 -0.12564300
H -4.87744500 2.35391500 -0.26305000
H -4.33128200 -1.26459800 -1.97669000
H -2.96518000 -0.11807500 -2.01176500
H -4.08829400 -1.52718800 0.47926600
H -2.49549600 -1.85108000 -0.31158600
H -3.28873300 2.01779500 -1.00429000

N -2.63135100 -0.02839200 0.71963600
O -4.73142000 0.53033300 -1.12683800
C -3.60852500 1.09808600 0.91728200
H -3.06683900 1.87452500 1.46757400
H -4.43398700 0.70201800 1.52322500
C -2.20912800 -0.57421000 2.03709500
H -3.10504300 -0.84201400 2.60675800
H -1.61968400 0.19357100 2.54550600
H -1.59709500 -1.46353900 1.86165400
C 3.13803000 2.14596700 0.75917900
H 2.08614500 2.21350600 0.45548500
H 3.15618900 1.98154300 1.84369900
H 3.62388700 3.10426600 0.53800100
O 0.68404900 0.48438600 1.51636100
H 2.88728100 1.49185000 -1.60320600
O 0.88452500 0.66085100 -1.45562200
H 2.05492200 -0.12668000 -1.21829700

14_{NMO•H2O}

C -4.16257800 -0.82597500 0.52866500
O -4.94938800 0.10277300 -0.19283500
Os -0.14761000 -0.03646000 -0.29978200
O -2.17124900 0.32977400 -0.11529500
C -2.93534800 -0.07769500 1.02434900
C -3.25943700 1.12972300 1.87671200
O 1.88132500 -0.19255200 -0.60458300
O 0.00424900 -0.05711100 1.46468000
H -4.70942700 -1.16930600 1.43113800
H -2.30916600 -0.77908500 1.59640400
H -3.84548100 0.83128200 2.75573300
H -2.33127600 1.60306700 2.21832000
H -3.84221600 1.86229100 1.30659300
C 4.59977900 0.32466500 -0.80683500
C 3.60368400 1.32344500 1.03155600
C 2.97567600 0.02953500 1.49147900
H 5.57283100 0.17798300 -1.28996000
H 3.83824900 1.94193800 1.90459400
H 2.89483200 1.87000800 0.38785200
H 3.65335300 -0.53485300 2.14677500
H 1.99904600 0.17817800 1.96586500
H 3.93422800 0.85778700 -1.50256600
N 2.71691300 -0.84957400 0.28501900
O 4.82106200 1.07671500 0.35918700
C 4.00694500 -1.02886800 -0.46775600
H 3.75655500 -1.61138900 -1.36085300
H 4.68105100 -1.59886100 0.18519500
C 2.16990200 -2.17078400 0.69340600
H 2.93824100 -2.71137000 1.25647700
H 1.89409500 -2.70704400 -0.21927100
H 1.28807300 -1.98799200 1.31447700
C -3.78615000 -2.02471900 -0.31981600
H -3.20143100 -1.70596200 -1.19116700
H -3.17679800 -2.73670700 0.25329800
H -4.68290400 -2.55921800 -0.66500100
O -0.45105500 -1.35247800 -1.37288600
H -5.63223000 -0.38924500 -0.66618200
O 0.07724900 1.67292300 -0.92077500
H -2.38234100 1.37111100 -0.46001900
O -2.18521500 2.59646900 -0.88545300
H -1.11887600 2.35830000 -0.95230100
H -2.50907900 2.66896600 -1.79399100

15

C -2.93916400 1.10193900 0.29588200
O -1.51892400 1.27792300 0.28930400
Os -0.47513100 -0.31727000 0.03365300
O -2.26539200 -1.08220400 -0.15771400
C -3.23658000 -0.13353200 -0.53067400
C -4.61502500 -0.71336400 -0.31600100
O 0.96813300 0.78241100 0.37938400
H -3.24697500 0.90291400 1.33961700
H -3.09450600 0.12879000 -1.60178300
H -4.71752400 -1.64902900 -0.87674600
H -4.76910200 -0.93591000 0.74816800
H -5.39824800 -0.02107000 -0.65148200
C 3.15868900 -0.80482700 -1.33889700
C 3.59094400 1.43594500 -1.02355000
C 3.46215800 1.32819100 0.48216100
H 3.56495000 -1.70883000 -1.80571900
H 4.30423000 2.22737300 -1.27921700
H 2.61085800 1.68560600 -1.46408000
H 4.45784300 1.17801200 0.93629600
H 3.00276700 2.22516500 0.91520200
H 2.18975100 -0.57393700 -1.81319600
N 2.62169400 0.18688600 0.85357300
O 4.08507900 0.23366300 -1.55903600
C 2.96842400 -1.04994300 0.14643100
H 2.17809200 -1.78681200 0.34306500
H 3.90923000 -1.42576500 0.58762400
C 2.49270200 0.02456800 2.29789500
H 2.06001500 0.94180000 2.70905600
H 3.48589200 -0.15110000 2.74279600
H 1.82050600 -0.81258800 2.50423900
C -3.56610700 2.37775200 -0.21195900
H -4.66127400 2.32481700 -0.15518500
H -3.23283500 3.23359000 0.38598500
H -3.27560100 2.55541000 -1.25589200
O -0.17858000 -1.33689300 1.40349400
O -0.00609100 -0.74171200 -1.56156800

15_{NMO}

C -0.42840400 2.39274800 0.32521200
O -0.19433000 1.11393000 0.82334200
Os 0.06232100 -0.38008200 -0.52272900
O -0.21145300 1.27633900 -1.69941000
C 0.18059200 2.44314700 -1.07874500
C -0.26705300 3.64122900 -1.89121200
O 1.88298600 -0.04758600 -0.50024800
O -2.06943500 -0.30535600 -0.56969400
H -1.52423300 2.55007800 0.19548900
H 1.29203200 2.47447000 -0.94555700
H 0.13747900 3.57902100 -2.90821400
H -1.36340400 3.65431600 -1.96494200
H 0.06985100 4.58513700 -1.44115000
C 4.54219400 0.73217300 0.09408200
C 3.27973100 0.38620900 2.00599500
C 2.95338200 -1.03836300 1.61686600
H 5.54219100 1.03504300 -0.23750600
H 3.33713400 0.46355500 3.09709900
H 2.48342400 1.05868800 1.64484900
H 3.72057500 -1.72468800 2.01906700

H 1.95017700 -1.33377900 1.93859500
H 3.80545400 1.44280800 -0.31238800
N 2.98815100 -1.18032400 0.14147500
O 4.54365000 0.76165200 1.49905800
C 4.24798700 -0.66759800 -0.42156000
H 4.15111100 -0.68454900 -1.51343300
H 5.04902900 -1.36079300 -0.11366500
C 2.65024400 -2.51621700 -0.33763900
H 1.72209600 -2.83266700 0.14655400
H 3.47235700 -3.20614700 -0.09188600
H 2.50354700 -2.47213600 -1.42188200
C 0.11793000 3.42504500 1.29129000
H -0.12257900 4.44654000 0.96666100
H -0.30502600 3.27515600 2.29270100
H 1.21134000 3.33285100 1.36789800
O 0.06338600 -1.43260800 0.93617300
C -3.24929000 0.44793900 1.95472400
C -4.65017700 0.52191400 0.11073200
C -4.26679600 -0.87979800 -0.31296100
H -3.25534100 0.57837800 3.04260200
H -5.69017800 0.71361500 -0.17877800
H -4.00048300 1.25113300 -0.39779300
H -4.92745600 -1.62124900 0.15636700
H -4.26665700 -1.00098900 -1.40121900
H -2.55375900 1.18103800 1.51942100
N -2.86420200 -1.18557500 0.13600500
O -4.57385400 0.65683600 1.50733800
C -2.77416000 -0.94725100 1.62972000
H -1.72099800 -1.10971200 1.88957900
H -3.42035400 -1.70399600 2.09673700
C -2.52518000 -2.59691900 -0.19162600
H -2.51848500 -2.68034600 -1.28190700
H -3.27464600 -3.25968500 0.25546100
H -1.52937500 -2.78879700 0.21744400
O 0.00343600 -1.33075200 -1.94911300

15NMM

C -2.87942800 -1.73471300 -0.57924000
O -2.64235900 -0.43930800 -0.11742800
Os -0.64427800 -0.04563600 0.06173100
O -0.58817900 -1.96202700 0.07099900
C -1.86009900 -2.63252000 0.13102300
C -2.21949400 -2.90531200 1.57584600
O -0.63991100 0.24165800 -1.65914400
O -1.03988900 0.32943500 1.71880700
H -3.89344500 -2.03552100 -0.24993600
H -1.71607900 -3.58056100 -0.41598400
H -1.41410000 -3.44994700 2.08580500
H -2.40135300 -1.96213600 2.10541600
H -3.13047300 -3.51607700 1.63131600
C 2.87693200 -1.73480500 -1.61632200
C 4.04086700 -0.11225700 -0.44928700
C 3.55977200 -0.65586000 0.88424700
H 3.00449000 -2.48651900 -2.40312600
H 5.04182400 0.31949200 -0.33501200
H 3.35405900 0.67873800 -0.79248600
H 4.32623300 -1.32982200 1.31321300
H 3.37571100 0.15970200 1.59672300
H 2.13891600 -0.98719700 -1.95840900
N 2.32217400 -1.40881600 0.73421100
O 4.13593200 -1.13436400 -1.41053700
C 2.38789400 -2.39336800 -0.34266100
H 1.39195000 -2.82777700 -0.47066700

H 3.10356300 -3.18624300 -0.04636000
C 1.78770500 -1.88128500 1.99392800
H 2.52864800 -2.51298700 2.51525800
H 0.87051800 -2.44606600 1.80795300
H 1.54206900 -1.01539700 2.62196200
C -2.81097200 -1.87360400 -2.09442400
H -3.13362500 -2.87793900 -2.40498800
H -3.47395100 -1.13688100 -2.56435500
H -1.79562700 -1.69848900 -2.46857000
C 0.94755500 3.13842000 1.25467100
C 1.12917300 3.06226600 -1.05354600
C -0.37242300 2.98576500 -1.21434600
C -0.56157800 3.05876600 1.18048500
H 1.56627400 3.60439800 -1.90015300
H 1.37319200 2.12523600 1.37479300
H 1.24143700 3.74290600 2.12117700
H -0.78441200 4.00587000 -1.31306000
H -0.64163900 2.40228000 -2.10137900
H -0.98116300 4.08025200 1.15150900
H -0.97139100 2.52847500 2.04688000
H 1.55281500 2.04134600 -1.03806400
C -2.47003100 2.47183200 -0.15939900
H -2.94317600 2.01847600 0.71653100
H -2.75191900 3.53469600 -0.23141500
H -2.80436300 1.92899100 -1.04837200
O 1.49075800 3.76380100 0.11417700
N -1.00789200 2.35096700 -0.03944800
O 1.14051300 0.19980500 0.28725800

16

C 2.74307000 0.07132700 0.74039000
O 1.45596200 -0.26242000 1.19461800
Os 0.04147800 -0.37732200 -0.13480400
O 1.34954300 0.74145000 -1.01753900
C 2.51055700 1.13611500 -0.32596500
C 2.31720300 2.52506700 0.24623200
O 0.15897000 -1.97430600 -0.69994900
O -1.03214400 -0.34907600 1.22910900
O -1.08558300 0.42690100 -1.19739800
H 3.28825300 0.50284500 1.59752700
H 3.33420800 1.12984500 -1.06090600
H 2.00129600 3.21971000 -0.53989900
H 1.54185700 2.50352100 1.02553200
H 3.24742800 2.89716800 0.69374800
C -3.21362900 0.07098300 0.66415200
H -3.17704300 0.30019800 1.72833300
C -3.03148500 1.08264100 -0.22806500
H -3.31307000 0.91573700 -1.26708800
C -2.65042500 2.46510600 0.16596200
H -2.31012300 2.49789200 1.20887200
H -1.84257300 2.83926800 -0.47665800
H -3.49562300 3.15940600 0.05547400
C -3.63438800 -1.29917100 0.26817100
H -2.99241800 -2.05486900 0.74044900
H -4.66391300 -1.50951800 0.59108800
H -3.57854000 -1.43045800 -0.81983700
C 3.47047700 -1.14880200 0.21286900
H 4.51127600 -0.89827400 -0.03007400
H 3.46777100 -1.94755300 0.96291700
H 2.98661200 -1.52842100 -0.69755800

17

C 2.59885200 0.03883700 0.78710500
O 1.27745200 -0.28940400 1.22999300
Os -0.00000200 -0.40649300 -0.17419400
O 1.25996800 0.72611100 -1.05505300
C 2.42815900 1.07632900 -0.31335200
C 2.25165300 2.48332000 0.21745800
O -0.00001000 -1.95158500 -0.83538300
O -1.27747500 -0.28943600 1.22998500
O -1.25993800 0.72616900 -1.05501700
H 3.10450400 0.48337300 1.65919600
H 3.27160400 1.03005500 -1.02208500
H 1.96489900 3.16064400 -0.59453300
H 1.45643700 2.49857400 0.97695500
H 3.17651100 2.85391000 0.67819500
C -2.59886300 0.03882400 0.78708500
H -3.10453600 0.48332500 1.65918300
C -2.42814100 1.07636600 -0.31332100
H -3.27157200 1.03013100 -1.02207400
C -2.25162900 2.48332900 0.21755600
H -1.45643100 2.49853500 0.97707300
H -1.96484600 3.16068800 -0.59439700
H -3.17649300 2.85391200 0.67828800
C -3.32598100 -1.21101700 0.33992900
H -3.27835100 -1.97872700 1.12049600
H -4.38073400 -0.98996500 0.13058500
H -2.87810100 -1.62341700 -0.57532900
C 3.32597500 -1.21102800 0.34002300
H 4.38073600 -0.98999200 0.13070500
H 3.27831300 -1.97870600 1.12061800
H 2.87812300 -1.62346000 -0.57523500

17_{H2O}

C 2.22515700 0.63474400 0.99390300
O 1.08702400 -0.23267100 1.16186400
Os -0.18330100 -0.22017700 -0.25328600
O 1.02545400 1.06622100 -0.97923500
C 2.36031600 0.89192300 -0.49006200
C 3.16052800 2.12003300 -0.84570800
O -0.10898100 -1.60179500 -1.21554800
H 1.96850800 1.58432400 1.49829200
H 2.78822400 -0.01346700 -0.95938400
H 2.73795000 3.00573800 -0.35345900
H 4.20865200 2.00911000 -0.54045100
H 3.13432200 2.28594700 -1.92822100
O -1.43394500 -0.52202100 1.16515400
O -1.51322000 1.00725100 -0.80700300
C -2.71611100 1.06394500 -0.02804700
H -3.54610100 1.09711000 -0.75210200
C -2.78004800 -0.21041800 0.80433800
H -3.31194600 -0.01669300 1.74969300
C -2.68209200 2.32485900 0.80703100
H -2.46746700 3.19484300 0.17687600
H -3.64324800 2.48473900 1.31232300
H -1.89741600 2.24814600 1.57275800
C -3.41630000 -1.37669900 0.07747000
H -3.31746900 -2.29405400 0.66871400
H -4.48362700 -1.18742300 -0.09680700
H -2.93846200 -1.54548400 -0.89819700
C 3.43195200 0.00236600 1.64458000
H 4.27438900 0.70601500 1.64788400

H 3.20654700 -0.25878800 2.68518000
H 3.73027900 -0.90506700 1.10537700
O 2.47148500 -2.63096300 -0.00501500
H 1.81928900 -2.79850500 -0.69796100
H 1.94552500 -2.25574300 0.71643400

17_{2(OH)}

C -2.72971400 -0.34815200 -0.68186300
O -1.43113700 -0.19820000 -1.25544400
Os -0.01154500 -0.00001000 -0.00000200
O -1.43112800 0.19818700 1.25544400
C -2.72970200 0.34818100 0.68186700
C -3.10639700 1.81660800 0.60521900
O 1.43896000 0.25131000 -1.24937400
O 1.43896000 -0.25134400 1.24936400
H -3.41103000 0.16954600 -1.37855200
H -3.41102300 -0.16950900 1.37855800
H -2.95712200 2.29823300 1.57786700
H -2.48298400 2.33399700 -0.13300700
H -4.16089700 1.92000300 0.31705000
C 2.73244100 0.37690000 -0.66470000
H 3.42496000 -0.10091700 -1.37862500
C 2.73245400 -0.37686700 0.66469900
H 3.42494300 0.10098100 1.37863300
C 3.11646800 -1.83872100 0.50532000
H 2.53720000 -2.31127900 -0.29968400
H 4.17946000 -1.92712800 0.24645600
H 2.95007200 -2.38546900 1.44230100
C 3.11638300 1.83877300 -0.50532200
H 4.17936400 1.92723200 -0.24643100
H 2.94998500 2.38550500 -1.44231200
H 2.53707000 2.31131000 0.29966200
C -3.10644900 -1.81656600 -0.60519800
H -4.16095600 -1.91993000 -0.31704100
H -2.95717100 -2.29820700 -1.57783800
H -2.48305400 -2.33395800 0.13304100
O -0.04050000 1.92263400 0.03064800
H 0.54434000 2.27568700 -0.65907000
O -0.04051000 -1.92265500 -0.03065500
H 0.54422000 -2.27571400 0.65915400

17_{NMO}

C 2.69924600 0.59609200 0.57644300
O 1.71968600 -0.22551300 1.18100200
Os 0.49248400 -1.05418500 -0.06012300
O 1.59786200 -0.26266000 -1.40144500
C 2.81950600 0.27082000 -0.91323600
C 3.17732200 1.48197400 -1.74374600
O 1.04242400 -2.64570900 -0.03517900
O -0.96619600 -1.14495000 1.24345900
O -0.97033200 -1.12378800 -1.30536400
H 2.35842300 1.64695800 0.66468500
H 3.58472400 -0.52228600 -1.03494000
H 3.26821600 1.21212900 -2.80176600
H 2.37393400 2.22575300 -1.64590300
H 4.12426700 1.93174600 -1.41432000
C -2.04183300 -1.88626700 0.68526000
H -1.73164200 -2.95130900 0.64131100
C -2.24059900 -1.40825400 -0.75004200

H -2.83475300 -0.47151900 -0.73976900
 C -2.92830400 -2.42577100 -1.63528000
 H -2.34889000 -3.35834800 -1.65296400
 H -3.94331100 -2.64631300 -1.27796700
 H -2.99696900 -2.04849700 -2.66166700
 C -3.26529200 -1.76679100 1.56578900
 H -4.06738200 -2.43058300 1.21767400
 H -3.01340600 -2.04591800 2.59533700
 H -3.65743500 -0.73982100 1.57858900
 C 4.00143200 0.42577900 1.32939100
 H 4.78472200 1.07595400 0.91607700
 H 3.86662200 0.67609800 2.38852000
 H 4.34138500 -0.61618700 1.26625400
 C -0.33770800 3.45712100 0.47866500
 C -2.19919200 1.90644200 0.69014300
 C -2.63073300 2.32172000 -0.69630300
 C -0.86945400 3.81775800 -0.89218400
 H -2.42278100 0.86074200 0.91718600
 H -0.77895300 4.10073700 1.25217600
 H 0.75574900 3.50797800 0.52301600
 H -2.17930400 1.64581000 -1.44050300
 H -3.72254300 2.26309100 -0.77617000
 H -0.37423900 3.19344700 -1.65168400
 H -0.65484300 4.87221900 -1.10086700
 H -2.64592000 2.56191600 1.45054800
 O -0.08608200 1.25226000 -0.13597500
 C -0.28578000 1.70695500 2.19959400
 H -0.78629200 2.40119300 2.88437700
 H -0.56863500 0.66971300 2.39567400
 H 0.79950800 1.80486700 2.26090300
 N -0.70066600 2.03100700 0.80315500
 O -2.26811700 3.66235100 -0.94318600

17_[ox]

C -2.87481000 -0.48584300 0.00251500
 O -1.88419900 -0.40345800 -0.98049000
 Os -0.00000100 -0.06636700 -0.26961700
 O -1.14131300 0.65359000 1.07502600
 C -2.56890400 0.71299900 0.88770900
 C -2.94326600 2.04603200 0.28531000
 O -0.00000800 -1.76894500 -0.04372000
 O 1.88420000 -0.40347400 -0.98048500
 O 1.14131200 0.65359100 1.07502400
 H -3.83485600 -0.32950500 -0.52316800
 H -2.98900100 0.60666700 1.90132700
 H -2.53920400 2.86613500 0.88917200
 H -2.55032600 2.12778600 -0.73543400
 H -4.03523400 2.15085000 0.24667700
 C 2.87481400 -0.48584200 0.00251900
 H 3.83485600 -0.32950300 -0.52316900
 C 2.56890300 0.71300700 0.88770200
 H 2.98900300 0.60668700 1.90132000
 C 2.94325500 2.04603600 0.28529000
 H 2.55031100 2.12777800 -0.73545400
 H 2.53919000 2.86614300 0.88914400
 H 4.03522300 2.15086000 0.24665200
 C 2.91767100 -1.79689200 0.76746400
 H 2.93321300 -2.64172400 0.06985800
 H 3.82117200 -1.83942700 1.39074900
 H 2.04588100 -1.91143100 1.42237000
 C -2.91765300 -1.79690300 0.76744400
 H -3.82114900 -1.83945200 1.39073500

H -2.93319300 -2.64172600 0.06982800
 H -2.04585600 -1.91144400 1.42234300
 O 0.00000700 0.92739600 -1.66382400

18

Os 0.76351400 0.04856200 -0.08774700
 O -0.79300500 -0.52507700 -1.06234300
 O -0.97976300 0.50193700 1.23599800
 C -2.13349000 -0.42841100 -0.64678200
 C -2.19158900 0.59922500 0.50676900
 H -2.68089900 -0.01162800 -1.51104600
 C -2.37384000 2.01888100 0.02346100
 H -3.00921400 0.31461800 1.19016900
 H -2.30454100 2.71808000 0.86379800
 H -1.59766700 2.28262300 -0.70755900
 H -3.35405800 2.14035600 -0.45506200
 O 0.78102900 1.60643600 -0.79357600
 O 1.79578800 -0.93524400 -1.01842200
 O 1.66245400 0.34314700 1.34269700
 C -2.69561000 -1.79402400 -0.30680100
 H -3.77094900 -1.71624700 -0.09996800
 H -2.55355200 -2.47804900 -1.15053300
 H -2.18872700 -2.22399200 0.56464500
 O 0.01479400 -1.58772400 1.18483900
 H -0.72589100 -0.60362100 1.51506300
 H 0.67522600 -1.71469000 1.88585300

18_{H2O}

Os 0.81790400 -0.15035100 0.03623200
 O -0.59748000 -0.51289700 1.29210200
 O -1.02372800 -0.00977300 -1.13642400
 C -1.96993300 -0.41839300 1.01949900
 C -2.14765800 -0.59679100 -0.50346400
 H -2.43688800 -1.28079500 1.52765800
 C -2.25375000 -2.04798400 -0.91300600
 H -3.04309800 -0.03569600 -0.82568200
 H -2.29024200 -2.13419400 -2.00426800
 H -1.38399900 -2.61380900 -0.55407900
 H -3.16021900 -2.50219600 -0.49211600
 O 0.97540500 -1.79399000 -0.42513500
 O 2.00443400 0.05820000 1.24446600
 O 1.46915700 0.63846400 -1.33587400
 C -2.55881200 0.86397100 1.57335500
 H -3.65107900 0.85709400 1.46074000
 H -2.31725000 0.96008600 2.63718500
 H -2.14225900 1.73888100 1.06399500
 O 0.17820900 1.89446600 0.52077600
 H -0.52822000 2.34239200 -0.52196200
 H 0.99842500 2.40866000 0.56606300
 O -1.17949400 2.35469500 -1.42084400
 H -2.03643100 2.73020800 -1.17543200
 H -1.20056900 1.11789600 -1.40657100

19

Os -0.78341600 -0.05515600 -0.06405300
 O 1.22332800 -0.56725300 1.27383600

O 0.76223100 0.51833000 -1.06145000
C 2.37562400 -0.47192400 0.41436500
C 2.07751200 0.65870100 -0.58366200
H 3.22589800 -0.16352500 1.04380900
C 2.38894300 2.04273600 -0.04251100
H 2.70975700 0.48189500 -1.47222300
H 2.00405900 2.80420600 -0.72884900
H 1.92678000 2.20361600 0.93484000
H 3.47759800 2.16190900 0.04083500
O -1.95809800 0.43539400 -1.19021300
O -1.64681500 -0.30710900 1.40242000
O -0.47237200 -1.71183600 -0.45218700
H 1.08995200 -1.50019800 1.50896900
C 2.67108900 -1.79048300 -0.26663000
H 3.60502200 -1.71603400 -0.83722300
H 2.80156100 -2.59793500 0.46743200
H 1.86272600 -2.06837600 -0.95350600
O -0.33831300 1.66439400 0.78918100
H -0.80242400 1.69674900 1.64187500

19_{H2O}

Os 0.88632400 -0.07075200 0.02187600
O -0.49204500 -0.59386300 1.25865900
O -1.13400900 -0.09272900 -1.19147600
C -1.87887500 -0.59698800 1.05365500
C -2.15770100 -0.77011600 -0.45678100
H -2.24391100 -1.50437500 1.56763600
C -2.17279800 -2.21901300 -0.88286900
H -3.11666500 -0.28297500 -0.69929000
H -2.28729700 -2.29691000 -1.96929800
H -1.23488700 -2.71250300 -0.60004100
H -3.00452300 -2.74837600 -0.40090600
O 0.97394200 -1.65155200 -0.64830100
O 2.14899300 -0.03982300 1.16083300
O 1.48122600 0.83555900 -1.30827400
C -2.54319200 0.61310700 1.68161500
H -3.63451000 0.49076600 1.66945200
H -2.21425500 0.72466400 2.72001300
H -2.27714100 1.52884700 1.14671200
O 0.09853600 1.75692300 0.54993400
H -1.24471500 2.48254900 -0.41365500
H 0.70873300 2.39628900 0.14446800
O -1.84638900 2.47713200 -1.19318100
H -2.71275000 2.75744100 -0.87310000
H -1.42535700 0.84658600 -1.35385100

20

Os 1.13463200 -0.02146600 -0.00872800
O -3.81075800 -0.14454300 -1.01349500
O -1.00265800 0.08031200 -0.42180300
C -3.28145500 -0.22874200 0.28781000
C -1.98551600 0.57647700 0.45318200
H -3.98869700 0.19710500 1.02910900
C -2.16391900 2.06028100 0.20282300
H -1.65278900 0.42518200 1.49998900
H -1.22696400 2.59533000 0.40392800
H -2.42350200 2.24435800 -0.84839700
H -2.94326300 2.48504500 0.84964100
O 0.67128400 0.57612600 1.52304100
O 1.39082900 1.25677100 -1.09904700

O 2.67158900 -0.70738400 0.27900100
O 0.44763800 -1.56048100 -0.70897900
H -4.03480100 0.77656200 -1.20068300
H -0.61650600 -1.12276500 -0.70766800
C -3.09213500 -1.69858600 0.58851100
H -2.65177200 -1.84683300 1.58270000
H -4.05670600 -2.21613500 0.55130800
H -2.44228000 -2.16942600 -0.16027100

20_{H2O}

Os -1.15882800 -0.04613500 0.05368700
O 3.62417700 0.52410800 -0.42641600
O 0.93572100 0.03992900 -0.34055600
C 3.10037700 -0.41402200 0.51030500
C 1.79559300 -1.01644000 -0.02088500
H 3.82570800 -1.23545500 0.66342900
C 2.01358600 -1.90166200 -1.23896400
H 1.36429400 -1.62933000 0.79491000
H 1.06098100 -2.31471200 -1.58907500
H 2.43578800 -1.31802900 -2.06996000
H 2.69087100 -2.73665800 -1.01167700
O -0.63693700 -0.55966800 1.60203300
O -1.17922000 -1.33293300 -1.07312600
O -2.83637600 0.14413700 0.36278800
O -0.94920200 1.63153500 -0.53199400
H 3.94075100 0.02899100 -1.19437100
H 0.19046500 2.17837100 -0.70207400
C 2.89689700 0.32702200 1.81090200
H 2.51768900 -0.35235400 2.58418600
H 3.83865900 0.76872600 2.15474100
H 2.16304800 1.13256400 1.68269900
O 1.30183100 2.41789700 -0.77437100
H 1.54469100 2.66875400 -1.67970200
H 1.57932800 1.42596700 -0.62831000

21

C 2.30336400 -2.28147000 -0.08948000
O 2.09713600 -0.99460900 -0.66008100
Os 0.63632200 -0.03577000 0.08986500
O 0.03239000 -1.92678400 0.45315200
C 0.92040300 -2.92796500 -0.00187300
C 0.44619500 -3.45883400 -1.34145100
O -1.30894200 0.49305200 -0.03754900
H 2.94441900 -2.83398300 -0.79693900
H 0.93969400 -3.74551200 0.74284700
H -0.58863900 -3.81990700 -1.26906000
H 0.48301800 -2.65480400 -2.09021400
H 1.07309600 -4.28920700 -1.69354000
C -3.93108500 1.15678600 -0.68113200
C -3.38819700 -1.02955700 -1.23225500
C -2.84678200 -1.32124700 0.14700000
H -4.77180300 1.85977600 -0.67186800
H -3.82396500 -1.94467100 -1.64833000
H -2.57117000 -0.69863600 -1.89408100
H -3.64395300 -1.67833000 0.81337300
H -1.99524900 -2.01112500 0.14199700
H -3.13892600 1.56167600 -1.32925200
N -2.32199200 -0.04522300 0.76386500
O -4.41782600 -0.06708100 -1.17489600
C -3.40633400 0.99634200 0.73144000
H -2.95386700 1.91822200 1.11284500
H -4.20016800 0.65042600 1.40658600
C -1.86517900 -0.27574900 2.15986400

H -2.73552200 -0.53880500 2.77124800
H -1.40387800 0.65330000 2.51005300
H -1.13353200 -1.08897400 2.14125400
O 1.26864500 1.07811900 1.23926700
O 0.72720100 1.22114300 -1.28687600
C 1.69990400 2.79563900 -1.00723100
H 1.05785500 3.23117700 -1.77559600
C 1.45884600 3.18092100 0.29859600
H 2.27860700 3.17754200 1.01570400
C 3.08207600 2.40646000 -1.43217000
H 3.04221700 1.72120900 -2.28510000
H 3.68437900 3.28366200 -1.71210200
H 3.59772100 1.88796100 -0.61202200
C 0.14964900 3.73807600 0.73931000
H -0.23877900 3.18719600 1.61155200
H 0.21807800 4.79615000 1.03836700
H -0.59336000 3.65244200 -0.06582600
C 2.99093400 -2.18141200 1.25775300
H 3.27957600 -3.17632200 1.62340000
H 3.89212700 -1.56148900 1.18247400
H 2.32388900 -1.72256200 2.00105000

22

C 2.71612900 -1.84807800 0.07938100
O 2.35664000 -0.59168700 -0.47628300
Os 0.62784300 0.03216200 0.02817000
O 0.35878200 -1.90194400 0.30371500
C 1.46545000 -2.72893100 -0.01387700
C 1.27713200 -3.31966800 -1.39660200
O -1.40011400 0.33549300 -0.07714800
H 3.52099900 -2.25912500 -0.55396700
H 1.52022100 -3.53702400 0.73875700
H 0.31164000 -3.83698500 -1.46593500
H 1.29514700 -2.51677900 -2.14621400
H 2.07230500 -4.03867900 -1.63513000
C -4.10948400 0.68469300 -0.59444600
C -3.33083900 -1.42018100 -1.18158200
C -2.68235600 -1.64082400 0.16554800
H -5.02617400 1.28381200 -0.55208300
H -3.67374600 -2.38167500 -1.57925800
H -2.59674000 -0.99028900 -1.88161700
H -3.38181200 -2.11368100 0.86887100
H -1.74493700 -2.20525400 0.10079500
H -3.39463000 1.17640200 -1.27255000
N -2.30326100 -0.30790800 0.76375500
O -4.46672100 -0.59106500 -1.06747100
C -3.51154400 0.58669000 0.79305200
H -3.16071600 1.55460600 1.16873700
H -4.22864100 0.14080500 1.49512500
C -1.76048800 -0.47851700 2.13892700
H -2.56834600 -0.81834800 2.79690100
H -1.36803000 0.49349100 2.45528600
H -0.95442600 -1.21642100 2.09380400
O 0.93566000 1.59814000 1.06748800
O 0.58935800 1.46311100 -1.38428200
C 1.24958400 2.64340200 -1.01213800
H 0.85271900 3.45411300 -1.65351700
C 0.85803700 2.88564400 0.43604200
H 1.58378000 3.52684300 0.96530100
C 2.75757700 2.55979200 -1.19487700
H 2.98959500 2.25742000 -2.22295200
H 3.23496500 3.53064800 -0.99686300

H 3.18858900 1.80940000 -0.52010300
C -0.54266400 3.44578500 0.59361200
H -0.86117100 3.39459500 1.64448900
H -0.58063300 4.49625900 0.27502700
H -1.24137400 2.86516700 -0.02254800
C 3.21528700 -1.68969500 1.50225600
H 3.61205900 -2.63954100 1.88665700
H 4.00906200 -0.93479400 1.54700500
H 2.39731700 -1.36099700 2.15883100

23

C -1.24927900 1.97126900 0.72977900
O -0.58611400 0.79156700 1.05687700
Os -1.23020800 -0.81611100 -0.00218700
O -1.63277500 0.71899300 -1.21453400
C -1.27908800 2.00381000 -0.79642300
C -2.25474200 3.00059600 -1.38441300
O -1.58571600 -1.83548700 -1.33470100
H -2.30153300 1.91790300 1.08397600
H -0.24386300 2.23738900 -1.13998600
H -3.26401700 2.81031500 -0.99739700
H -1.96590400 4.03032300 -1.13611300
H -2.28567600 2.90450700 -2.47527600
O -0.23053800 -1.76458600 1.03168200
O -2.73737700 -0.76180400 0.81636500
C -0.54568400 3.15533100 1.35610500
H -1.09589000 4.08917400 1.18270700
H -0.45097400 3.01258800 2.43929200
H 0.46436400 3.27051400 0.93281500
O 0.69075900 -0.50103800 -0.95671400
H 0.49553800 0.12444800 -1.66974400
N 2.47245300 0.00276900 0.76259000
C 3.13989300 1.28388900 0.43087200
C 3.35055500 -1.15365100 0.44117900
C 2.04372000 -0.02806200 2.17431000
C 3.64167000 1.25433200 -0.99945600
H 3.97752400 1.42502600 1.13087400
H 2.40418600 2.08523700 0.58687400
C 3.84462100 -1.05290500 -0.98744600
H 2.75265800 -2.06063200 0.59417600
H 4.19473000 -1.14456400 1.14764800
H 2.92678600 0.06808200 2.82019800
H 1.52334400 -0.97206900 2.35936200
H 1.33362400 0.78627500 2.34036100
H 4.20070200 2.17052700 -1.21973200
H 2.78379100 1.20012900 -1.69516400
O 4.51269100 0.17230300 -1.20164700
H 4.56627700 -1.85136500 -1.18966400
H 2.99219900 -1.15980500 -1.67887100
H 1.58330400 -0.10617900 0.04609700

24

C -1.09953600 1.97385900 0.76073700
O -0.42037800 0.78803100 1.02279700
Os -1.22041600 -0.80404200 -0.00911000
O -1.66216800 0.76227000 -1.16851500
C -1.23854600 2.02818500 -0.75895800
C -2.21809600 3.06541700 -1.26528300
O -1.75619900 -1.80301600 -1.29533700
H -2.12418100 1.92237500 1.18876900
H -0.22189600 2.23308900 -1.17103200

H -3.20178600 2.91021700 -0.80351100
H -1.87169700 4.08165000 -1.03474400
H -2.33557500 2.97940000 -2.35116200
O -0.19377700 -1.80556300 0.94861300
O -2.64043100 -0.65251600 0.94622300
C -0.35860400 3.15744700 1.34649700
H -0.96421200 4.07165500 1.29860400
H -0.11512800 2.96868000 2.39954300
H 0.57828400 3.34623500 0.79913700
O 0.60812100 -0.54451700 -1.06283900
H 0.38323900 0.08195500 -1.76640600
N 2.42846700 -0.11571200 0.77297000
C 3.04959700 1.21169800 0.51852500
C 3.31842300 -1.22163800 0.31344500
C 2.06539500 -0.27052400 2.19952700
C 3.48697200 1.31043600 -0.92882500
H 3.91331000 1.30930100 1.19180600
H 2.29827200 1.96975900 0.77519400
C 3.75209500 -0.98238200 -1.11870000
H 2.74335500 -2.15069900 0.40737900
H 4.18400800 -1.24968300 0.99101200
H 2.97412800 -0.16642000 2.80498500
H 1.60954800 -1.25421700 2.33651800
H 1.32056500 0.49131200 2.44425700
H 4.01039300 2.25857800 -1.09466400
H 2.60019400 1.28555400 -1.58821200
O 4.37901500 0.27513400 -1.25142600
H 4.48433300 -1.74045800 -1.41594400
H 2.87309400 -1.05494500 -1.77976200
H 1.55444200 -0.16972700 0.13185400

25

C -0.06642900 1.94713100 0.81737000
O 0.20283700 0.57333300 0.90184500
Os -1.46680600 -0.55636900 -0.00094800
O -1.60404800 1.24915700 -0.82638100
C -0.59720300 2.19380100 -0.59264900
C -1.17612800 3.57713200 -0.80193200
O -2.74260300 -1.17675600 -0.95323400
H -0.88719000 2.17862800 1.52293600
H 0.24956700 2.02399100 -1.29644500
H -1.95137400 3.77720600 -0.05076400
H -0.39668200 4.34656900 -0.72502300
H -1.63648200 3.65174900 -1.79314100
O -0.62133400 -1.92340000 0.61685100
O -2.29995800 0.01567400 1.39330700
C 1.14509600 2.78155100 1.17204500
H 0.88129800 3.84261800 1.26180500
H 1.55599900 2.45799500 2.13798600
H 1.93046800 2.69608200 0.40529900
O -0.11906800 -0.69516300 -1.48797100
H -0.37190100 -0.01936300 -2.13612500
N 2.39018300 -0.61412800 0.75895100
C 3.59419200 0.24639200 0.81472300
C 2.53144200 -1.63075300 -0.32055700
C 2.15797900 -1.26414400 2.06347500
C 3.91102300 0.81144600 -0.55576000
H 4.43752900 -0.36943600 1.16581000
H 3.41285700 1.04255000 1.54920000
C 2.91609000 -0.96482500 -1.62278400
H 1.56981000 -2.14713500 -0.41819300
H 3.31285100 -2.34003500 -0.00332600

H 3.02012300 -1.89116300 2.32795700
H 1.24811000 -1.86799800 1.99414500
H 2.01178900 -0.48711700 2.82167500
H 4.83196600 1.40450300 -0.51283200
H 3.08790900 1.47676100 -0.88670500
O 4.10640000 -0.21536100 -1.48677000
H 3.09332000 -1.72377900 -2.39195800
H 2.08436700 -0.32036300 -1.95178500
H 1.38748600 0.04442900 0.63408100

26

C -0.00598100 1.97942400 0.86633800
O 0.15819700 0.57700100 1.06656200
Os -1.59336800 -0.52674600 -0.01835400
O -1.55320200 1.29556000 -0.79624900
C -0.48063900 2.17088200 -0.57109300
C -0.94698100 3.58037500 -0.86903700
O -2.86761800 -1.11376400 -0.98249500
H -0.82556700 2.27333800 1.53944700
H 0.37212700 1.91093000 -1.23726000
H -1.72310800 3.88247100 -0.15410900
H -0.11217900 4.29039500 -0.81375300
H -1.37468300 3.62988400 -1.87600300
O -0.83599900 -1.90552900 0.66040200
O -2.40952900 0.12460800 1.34856300
C 1.26260900 2.72240100 1.21096700
H 1.10088000 3.80659500 1.19454200
H 1.60194900 2.44465700 2.21654100
H 2.06391100 2.48448100 0.49541600
O -0.16185900 -0.70349500 -1.38556100
H -0.30830600 -0.00954500 -2.04813900
N 2.56962200 -0.66957900 0.73748300
C 3.83727400 0.05565000 0.82971700
C 2.62936000 -1.63059600 -0.37124600
C 2.28458000 -1.35744400 1.99218600
C 4.18795900 0.69300900 -0.50068100
H 4.64995500 -0.63933600 1.12281900
H 3.75309400 0.82249000 1.61505200
C 3.00806000 -0.91951100 -1.65071000
H 1.64476000 -2.10315900 -0.48148400
H 3.38188400 -2.41314400 -0.14701800
H 3.08299000 -2.07734900 2.24989600
H 1.33175200 -1.89425300 1.90575300
H 2.19482600 -0.62185700 2.80246000
H 5.16862100 1.18059600 -0.44639800
H 3.43210700 1.46556800 -0.75363000
O 4.25086700 -0.26214900 -1.52500100
H 3.10251900 -1.63175300 -2.47759800
H 2.21678800 -0.18976400 -1.90374600
H 1.04999200 0.24552600 0.72130700

27

C -0.93607600 2.88899400 -0.40489400
O -0.39963000 2.35051400 -1.59726000
Os -1.02738800 -1.12940900 -0.17849900
O -0.86124500 0.75823700 0.65609000
C -1.73184200 1.83263900 0.35857000
C -2.32770200 2.35425600 1.65226400
O -1.54168900 -1.42740800 1.70402000
H -0.10618500 3.21564400 0.26174400
H -2.54612000 1.49142700 -0.30849700

H -1.54250500 2.75317900 2.31218000
H -3.06623400 3.14627000 1.47681200
H -2.83700600 1.53820900 2.18145600
O -2.56654100 -0.65944000 -0.76194600
O -1.05877800 -2.83273500 -0.32786200
C -1.75650700 4.10022300 -0.79311200
H -2.03543200 4.70400800 0.07881700
H -1.17269000 4.73036000 -1.47403000
H -2.66948100 3.79162500 -1.32077800
O 0.86000200 -1.28386800 0.81749800
H 1.65279700 -0.21428700 0.78491000
N 2.45767000 0.64726000 0.85146200
C 2.60363200 1.34685400 -0.45295000
C 3.73043600 -0.01851500 1.22264700
C 1.98129300 1.54853700 1.91165100
C 3.11915300 0.37578600 -1.49463400
H 3.32186900 2.16977600 -0.30798400
H 1.63104700 1.76571300 -0.74389000
C 4.18577300 -0.91960600 0.09047000
H 3.55083000 -0.59462200 2.14049900
H 4.48214600 0.75953900 1.42857500
H 2.64228300 2.42121300 1.99550300
H 1.97543800 1.00254500 2.86250000
H 0.95630600 1.84726400 1.66671700
H 3.29216000 0.90189400 -2.43922200
H 2.36899700 -0.41533500 -1.66813000
O 4.35137400 -0.18419100 -1.09393700
H 5.15346000 -1.37095400 0.33646800
H 3.44612800 -1.72809100 -0.05189800
H -0.28999000 1.38987500 -1.49189000
O 0.01889700 -0.59554300 -1.45307300
H -1.55169600 -0.52872800 2.07925600
H 0.59356600 -1.53179600 1.71824100

28

C 1.64841100 2.53013100 -0.35113400
O 1.54376400 2.06491800 -1.67583800
Os -1.68439900 -0.29081200 -0.21673000
O 0.32253600 0.63005300 0.14535800
C 0.47526300 1.98304900 0.47348300
C 0.67164400 2.18516900 1.96560900
O -2.20304300 0.92719000 1.28750000
H 2.58752600 2.13749000 0.10754500
H -0.42353400 2.54074300 0.14409500
H 1.63654500 1.76311700 2.29384900
H 0.66917100 3.24756400 2.24361700
H -0.13574500 1.68383700 2.51129800
O -1.86387600 1.09243500 -1.22439000
O -3.22123800 -1.02450000 -0.37274700
C 1.71672000 4.04042300 -0.37113600
H 1.90441100 4.45286100 0.62863900
H 2.52331200 4.37151200 -1.03568700
H 0.77409600 4.45301300 -0.75537200
O -1.15559000 -1.23726100 1.42327200
H 1.35130700 -0.38742300 0.61761300
N 2.08179400 -1.13419300 0.96423900
C 3.45212300 -0.57680200 0.78111900
C 1.91126600 -2.37683900 0.15148600
C 1.77822100 -1.38096100 2.38822300
C 3.76364200 -0.41727500 -0.69503200
H 4.15478200 -1.28234500 1.24846200

H 3.49758400 0.38237200 1.31377000
C 2.31625700 -2.11099400 -1.28380300
H 0.85970200 -2.67573900 0.22749400
H 2.55740700 -3.14536400 0.60088800
H 2.48350800 -2.11881100 2.78906000
H 0.74636500 -1.73957500 2.45133500
H 1.87402800 -0.43682000 2.93549900
H 4.79812400 -0.07607100 -0.81400800
H 3.09808300 0.33595800 -1.15698700
O 3.64714800 -1.65508900 -1.35280400
H 2.25388300 -3.03908800 -1.86184400
H 1.62483600 -1.37862000 -1.73419900
H 0.97427500 1.27475200 -1.60750400
O -0.67458600 -1.38422600 -1.08582000
H -2.48361700 1.77608400 0.91163900
H -1.44646400 -0.66193100 2.15344500

29

C 1.70773400 2.49211400 -0.36526400
O 1.56060700 2.04578900 -1.69196500
Os -1.70534800 -0.26756200 -0.21179300
O 0.36953900 0.59264100 0.15167200
C 0.55748700 1.94484500 0.48863700
C 0.79284700 2.12636300 1.97628000
O -2.15106300 0.94702600 1.31621200
H 2.65925000 2.09338000 0.05918100
H -0.34624100 2.50769200 0.18900200
H 1.75967300 1.68808100 2.27526300
H 0.81076200 3.18547300 2.26479800
H -0.00951900 1.63002600 2.53507100
O -1.82531000 1.14358100 -1.18924200
O -3.26829900 -0.93484600 -0.38080600
C 1.77850300 4.00274900 -0.36935800
H 2.00234700 4.40348000 0.62765200
H 2.56226700 4.33903500 -1.05798100
H 0.82439200 4.42178400 -0.71658400
O -1.19136300 -1.25002000 1.40184000
H 1.29017700 -0.32560900 0.59702000
N 2.05708500 -1.13697200 0.95320300
C 3.43679100 -0.61325500 0.77516100
C 1.86596500 -2.37161200 0.14041300
C 1.76399300 -1.39886600 2.37266100
C 3.76457100 -0.46222600 -0.69867500
H 4.12890500 -1.32939600 1.24506800
H 3.50535000 0.34652500 1.30571100
C 2.28318100 -2.12268000 -1.29383600
H 0.80908700 -2.65425900 0.20978500
H 2.49218200 -3.15940400 0.58791100
H 2.46427300 -2.14825000 2.76463600
H 0.73205300 -1.75537600 2.44523000
H 1.87113200 -0.46576900 2.93676200
H 4.80813100 -0.14653500 -0.80994800
H 3.12190600 0.30525900 -1.16879900
O 3.62415400 -1.69620300 -1.35884400
H 2.20443000 -3.05225700 -1.86766000
H 1.61247200 -1.37769000 -1.75491900
H 0.99296400 1.25543500 -1.62504100
O -0.73477600 -1.37086600 -1.10894400
H -2.41309100 1.80963900 0.95830900
H -1.45037500 -0.67916600 2.14786800

30

C 2.25930700 1.04031500 0.42202300
O 1.04648600 0.73725700 1.10742500
Os -0.24508900 -0.56053500 -0.08327900
O 1.32165700 -0.34972400 -1.19844000
C 2.54018600 -0.12373400 -0.52577000
C 3.60451400 0.17350100 -1.55749600
O -0.83681100 -2.07547600 -0.51696800
H 2.05980300 1.93355200 -0.19710100
H 2.82575500 -1.00910000 0.07581800
H 3.34072200 1.07725100 -2.12257900
H 4.58496800 0.32025500 -1.08612100
H 3.68524200 -0.65813600 -2.26596100
O -1.54254200 0.13458500 1.15124600
O -0.92528800 0.79596100 -1.19875700
C -1.99077000 1.58728000 -0.65497500
H -2.71945200 1.72142100 -1.47111500
C -2.61606100 0.80610300 0.49721000
H -3.04081300 1.50676000 1.23469700
C -1.40522600 2.91752000 -0.23014500
H -0.85478200 3.37342400 -1.06082200
H -2.19760000 3.60811200 0.08619200
H -0.71282700 2.76465300 0.60862500
C -3.67779500 -0.17852700 0.04892900
H -3.99213200 -0.80646000 0.89057600
H -4.55860800 0.35281200 -0.33496800
H -3.30491200 -0.83699500 -0.74744300
C 3.35795600 1.30622100 1.42413100
H 4.27740100 1.63812800 0.92563900
H 3.05016100 2.08558800 2.13040100
H 3.58560300 0.39488700 1.99633000
O 0.80041000 -1.49102200 1.55733000
H 0.12864100 -1.70061500 2.22747000
H 1.12559600 -0.34962300 1.68145000

30_{H2O}

C 2.38510500 0.62304300 0.84227500
O 1.09067900 0.23261200 1.29489900
Os -0.19995600 -0.32360600 -0.40214500
O 1.48900100 0.07399900 -1.24140900
C 2.65090700 -0.12738800 -0.46350900
C 3.83468300 0.40425700 -1.23879200
O -0.93439600 -1.41229000 -1.45810500
H 2.32706700 1.69998100 0.60201500
H 2.78651100 -1.20104300 -0.23580200
H 3.71669400 1.48080800 -1.41977400
H 4.77228200 0.23442400 -0.69401300
H 3.90714000 -0.09812500 -2.20962200
O -1.56913500 0.01024500 0.93572800
O -0.57157500 1.47731300 -0.84295400
C -1.57418800 2.13793000 -0.06491400
H -2.15622000 2.74985100 -0.77370000
C -2.45602100 1.06244300 0.56082300
H -2.90484200 1.44091700 1.49346500
C -0.87847200 3.01144000 0.95824200
H -0.16621200 3.68027900 0.46180000
H -1.60543000 3.62129300 1.50995800
H -0.32970600 2.37891500 1.66861600
C -3.53712700 0.55107600 -0.37039600
H -4.03890300 -0.32080900 0.06874900

H -4.29422900 1.32566800 -0.54856900
H -3.12009800 0.25341200 -1.34210400
C 3.40503100 0.36078800 1.92544900
H 4.39455400 0.73736500 1.63744500
H 3.10769200 0.85447900 2.85746500
H 3.48904200 -0.71809600 2.12055000
O 0.60983000 -1.91983200 0.70799100
H -0.15239900 -2.36578600 1.15679800
H 1.02039000 -0.96566900 1.35847600
O -1.89391500 -2.66885600 1.56459000
H -2.05796100 -1.70485000 1.55441000
H -2.24214900 -2.97599900 0.71590600

31

C 3.08971900 1.26832200 0.31931700
O 4.04132000 0.84438900 -0.63275700
Os -0.41337400 -0.68666100 -0.22449700
O 1.47519800 -0.41498200 -0.25198300
C 2.22152800 0.11956900 0.83482300
C 3.01939600 -1.02031800 1.43741900
O -0.73196900 -2.15203500 0.53260300
O -0.54229500 0.78049000 0.99788500
O -2.01681900 0.10204000 -0.88666600
H 3.59554600 1.69448100 1.21023800
H 1.54001900 0.53669400 1.59196800
H 2.34678500 -1.78059400 1.85378900
H 3.63241700 -1.50983200 0.66918100
H 3.67252600 -0.66175800 2.24521400
C -1.87614800 1.27112500 1.18089400
H -1.77080700 2.31213200 1.52600300
C -2.53646100 1.23169600 -0.19119300
H -3.62122800 1.06385200 -0.08544000
C -2.26721700 2.46826300 -1.02127600
H -1.18508200 2.65362500 -1.07885800
H -2.64483000 2.33156300 -2.04022100
H -2.74789600 3.35181800 -0.58139500
C -2.59161600 0.44039100 2.22420200
H -2.00695700 0.39929300 3.15031700
H -3.57541200 0.87078500 2.45193700
H -2.74512000 -0.58841600 1.86842100
C 2.25901200 2.34567400 -0.33998100
H 1.46935500 2.69657700 0.33677400
H 2.89106300 3.19314100 -0.62707600
H 1.78959600 1.94576000 -1.24854200
O -0.06448900 -0.95337800 -2.07014700
H 4.66968700 0.25317300 -0.19805700
H 0.90993100 -0.97654900 -2.15920500

31_{H2O}

C 3.40437900 0.87235300 -0.46108800
O 2.78732000 2.00799000 0.14583400
Os -0.44744700 -0.56829200 0.01204100
O 1.30223900 -0.12322300 -0.69179400
C 2.54790000 -0.32762900 -0.07527200
C 3.12558100 -1.65762800 -0.52395200
O -0.85663700 -1.90980700 -0.91169800
H 3.34744400 0.96071500 -1.56080400
H 2.47337700 -0.29602900 1.03029000
H 3.32578100 -1.63899100 -1.60388300
H 4.05227300 -1.91191800 0.00542400
H 2.39298100 -2.45440900 -0.33888100

O -1.99924500 -0.09840300 1.03414400
O -0.98253100 0.97988000 -0.99580900
C -2.26556800 1.51164100 -0.71794400
H -2.81647300 1.53011000 -1.67512200
C -2.98971000 0.57533800 0.26356000
H -3.58766700 1.16920200 0.97594900
C -2.12792600 2.92968900 -0.19976600
H -1.47300500 3.51494100 -0.85530300
H -3.10534200 3.42627300 -0.14523700
H -1.70068100 2.93920600 0.81329800
C -3.88258200 -0.43154600 -0.43266600
H -4.28157100 -1.15153200 0.29076300
H -4.72401800 0.07505200 -0.92430000
H -3.32578000 -0.98814400 -1.19926600
C 4.84500900 0.76266600 -0.00452300
H 5.37808600 -0.04068400 -0.52731600
H 5.38388500 1.69905500 -0.20150900
H 4.89062400 0.57213100 1.07668100
O 0.16916500 -1.42001500 1.61947700
H 1.13776000 -1.44065000 1.66277100
H 3.15625800 2.80595200 -0.25360900
H -0.30339500 1.79253800 1.70975800
O 0.43292400 1.24325400 1.41013300
H 1.01708100 1.78069800 0.83277300

31_{NMO}

C -3.36153800 -1.84124000 0.74477000
O -4.24291300 -0.82545900 0.30512300
Os 0.49207700 -0.95027700 -0.50222700
O -1.40833800 -0.84152800 -0.16226200
C -1.95870600 -1.30331400 1.05500800
C -1.97724200 -0.22850200 2.12918000
O 0.24655300 1.31144200 0.17115700
O 0.95635600 -0.87490800 1.35886200
O 2.27037900 -0.24927300 -0.74894200
H -3.73423900 -2.28723700 1.68974000
H -1.36770600 -2.15890300 1.43312000
H -0.96006300 0.13454300 2.30926700
H -2.59550400 0.63173900 1.83478800
H -2.37944100 -0.63789300 3.06711100
C 2.34468100 -0.71944100 1.60675700
H 2.78880200 -1.73454900 1.65168500
C 2.98173700 0.03204800 0.44070600
H 2.88192000 1.11726400 0.64376900
C 4.43897800 -0.31571400 0.22733300
H 4.54417100 -1.38781800 0.01567300
H 4.84332300 0.24098400 -0.62613000
H 5.03916500 -0.07260900 1.11474600
C 2.51068000 -0.00643200 2.92957100
H 2.05042900 -0.58360900 3.73967000
H 3.56924600 0.15401100 3.17503800
H 2.00661500 0.96982200 2.87549700
C -3.33855700 -2.90306300 -0.33079100
H -2.63393600 -3.70442300 -0.07275600
H -4.33630300 -3.33620100 -0.46435000
H -3.02106900 -2.46102400 -1.28179200
O -0.03343600 -0.23585700 -2.22704100
H -4.40637600 -0.22763900 1.04625200
H -1.00650800 -0.31733400 -2.23043700
C -2.26114200 2.52358900 -0.48423900
C -1.07081500 2.54552300 -1.40890900

C 0.21516500 3.59003600 0.36625700
C -1.02776800 3.52546500 1.22891800
H -1.05357700 1.70778100 -2.10881100
H -2.31900700 1.54271000 0.01012800
H -3.17716500 2.67239900 -1.06687200
H 1.13143500 3.47560600 0.95693700
H 0.24921200 4.52190600 -0.21522600
H -0.99805200 2.60561700 1.83292100
H -1.04884200 4.39165500 1.90067700
H -1.01855900 3.49553200 -1.95842900
O -2.19533800 3.58625200 0.44606000
C 1.37266600 2.52532800 -1.52341800
H 1.30551000 3.45440000 -2.10130100
H 2.27864600 2.51508500 -0.91206900
H 1.34767200 1.64358100 -2.16798400
O 0.65396300 -2.59034500 -0.84232800
N 0.20510600 2.43819200 -0.60193500

32

C -3.66492700 0.11531900 0.89897700
O -4.51065000 0.43564300 -0.18003000
Os 0.45435500 -0.23506300 -0.58716500
O -1.62792500 -0.08712700 -0.38168900
C -2.23225600 0.61956800 0.70289400
C -2.16087400 2.10208000 0.41649600
O 0.53105100 0.40879200 -2.14484600
O 0.85289100 0.95747300 0.83831300
O 2.19999600 -0.89398000 -0.23007900
H -4.01724700 0.60315000 1.83138100
H -1.67615900 0.39115300 1.63271000
H -1.11941700 2.44183800 0.41218300
H -2.59434000 2.31768900 -0.56881700
H -2.70122900 2.67345800 1.18404400
C 2.25908200 1.06101000 1.14330600
H 2.31010700 1.31219700 2.21437100
C 2.87615100 -0.30311200 0.88343300
H 3.93064400 -0.19460100 0.58093800
C 2.75893500 -1.25130800 2.05884400
H 1.71246100 -1.32106400 2.38635900
H 3.08966800 -2.25413400 1.76866500
H 3.36872900 -0.90647500 2.90410900
C 2.86336700 2.16932100 0.30898600
H 2.29445400 3.09791000 0.43131600
H 3.90319700 2.35666200 0.60611100
H 2.85861400 1.89953000 -0.75721700
C -3.73488700 -1.38576800 1.07397100
H -3.01737500 -1.73650700 1.82769100
H -4.74237100 -1.68487100 1.38187300
H -3.51985800 -1.88415500 0.12054400
O -0.24927600 -1.84414700 -0.13128100
H -4.58591500 1.39681000 -0.24234300
H -1.38117200 -1.21966500 -0.17389600

32_{NMO}

C 3.14815000 -2.74418200 -0.38862100
O 2.52297100 -3.82443000 0.27402400
Os 0.28325700 0.44456100 -0.13736600
O 1.31294000 -1.41603200 0.31146400
C 2.74035300 -1.42865000 0.27938200
C 3.29633100 -1.28911400 1.68124700

O -1.35208200 -0.93275900 -0.44419000
O 1.78553400 1.58342300 0.24171000
O -0.71451500 2.09681100 -0.11997400
H 4.23148200 -2.88624100 -0.24396800
H 3.09019300 -0.58952800 -0.34614200
H 2.95168000 -0.35721100 2.14821500
H 2.97661800 -2.14121300 2.29546700
H 4.39413600 -1.27581900 1.66366600
C 1.42043100 2.92365100 0.56576900
H 2.23829100 3.56661100 0.19876400
C 0.13204600 3.25675200 -0.17711300
H -0.41271700 4.06246800 0.34215700
C 0.36397100 3.63343400 -1.62666700
H 0.95186000 2.85950500 -2.13760300
H -0.59296100 3.74635400 -2.15210200
H 0.90962700 4.58329200 -1.69890600
C 1.28984700 3.06348300 2.07082100
H 2.19598600 2.68863500 2.56131500
H 1.14795200 4.11520800 2.35426100
H 0.43834000 2.47934200 2.44189000
C 2.82103400 -2.75156000 -1.87044800
H 3.36087000 -1.95838500 -2.40605000
H 3.08635900 -3.71974100 -2.31127000
H 1.74614200 -2.58170200 -2.01938200
O 0.06418900 -0.06101300 1.61670700
H 1.58713500 -3.56655000 0.31809500
H 0.73453100 -0.99882500 1.36951800
C -3.50508300 -2.52868300 0.40423100
C -3.47042900 -1.70648400 -0.86600900
C -3.16627200 0.27063700 0.54862500
C -3.21301400 -0.65979500 1.73866900
H -3.00520500 -2.24244100 -1.69987300
H -2.49249200 -2.89114200 0.63875200
H -4.16366500 -3.39200100 0.25589800
H -2.50467600 1.12909900 0.70252900
H -4.17410700 0.61599000 0.27971500
H -2.19046900 -0.96586900 2.00821100
H -3.65818700 -0.13347300 2.58998200
H -4.47987100 -1.37194500 -1.13970500
O -4.03327900 -1.77628700 1.46705400
C -2.68991500 0.38859100 -1.87031100
H -3.73596600 0.61640900 -2.10282800
H -2.13065000 1.30465700 -1.65574300
H -2.21258800 -0.16922800 -2.68024400
O 0.61565000 0.13313700 -1.78137300
N -2.63301700 -0.47202600 -0.65651800

32_{NMO·H2O}

C 3.25839500 -2.53150600 -0.63216400
O 2.68912000 -3.69282100 -0.05366100
Os 0.27528100 0.50496600 -0.11720900
O 1.33166400 -1.33496000 0.04738800
C 2.75241600 -1.28545400 0.09713200
C 3.24929200 -1.20697500 1.52727900
O -1.34720700 -0.87269600 -0.53166200
O 1.76417300 1.62002800 0.36113500
O -0.71195900 2.17919500 -0.12705900
H 4.34209100 -2.62225300 -0.45581000
H 3.07919500 -0.38898200 -0.45546500
H 2.77382500 -0.37087400 2.05620000
H 3.04493600 -2.14966600 2.05417100

H 4.33546600 -1.04859400 1.54972600
C 1.39747600 2.96693500 0.66771600
H 2.24286600 3.59927400 0.34687800
C 0.15340100 3.31854800 -0.14078600
H -0.39803600 4.13608200 0.35408500
C 0.47114400 3.70726900 -1.57255700
H 1.08385000 2.93788300 -2.05996200
H -0.45455900 3.82792100 -2.14992900
H 1.02184900 4.65691000 -1.60409300
C 1.18898900 3.09993400 2.16427400
H 2.07484300 2.73970300 2.70120900
H 1.01427800 4.14799200 2.44318400
H 0.32830700 2.49875300 2.48340700
C 2.97738700 -2.46106900 -2.12044800
H 3.51191300 -1.62329100 -2.58791000
H 3.28266700 -3.39222100 -2.61224100
H 1.90390300 -2.29980300 -2.29160200
O -0.19473200 0.10564500 1.60555300
H 1.73853800 -3.63857200 -0.23851800
H 0.81306700 -1.95558800 0.98213200
C -3.56000000 -2.46222200 0.16652900
C -3.43531900 -1.62949600 -1.09128200
C -3.21749000 0.33186900 0.36330800
C -3.38074500 -0.61048500 1.53424000
H -2.91572700 -2.15710900 -1.89787800
H -2.56530700 -2.81010800 0.48727300
H -4.19442200 -3.33231500 -0.03817300
H -2.55583400 1.17699500 0.58160200
H -4.19511600 0.69976100 0.02200800
H -2.39439900 -0.93805300 1.89383000
H -3.89219500 -0.08415800 2.34800100
H -4.42329700 -1.28940700 -1.42944600
O -4.18414500 -1.71602000 1.18325900
C -2.59266400 0.47982400 -2.01423100
H -3.62371200 0.71895700 -2.29724400
H -2.03782000 1.38755600 -1.75492600
H -2.07664000 -0.06798800 -2.80677700
O 0.56289100 0.34390500 -1.79554000
N -2.60988100 -0.40152100 -0.81259100
O 0.13165600 -2.22690400 1.89881000
H -0.13469200 -1.03458700 1.92827200
H 0.71257700 -2.43697100 2.64420800

33

C -0.92801100 2.26597300 0.99209200
O -0.45760700 0.95153800 1.00790000
Os -0.84791000 -0.17693800 -0.60527200
O -1.78372500 1.49136700 -1.04063300
C -1.24215000 2.63809000 -0.46377800
C -2.22887900 3.77724500 -0.60101400
O -0.71603900 -0.84710900 -2.15652900
H -1.88676400 2.30503000 1.55303700
H -0.28477900 2.93516800 -0.95436600
H -3.17581200 3.50414300 -0.11806200
H -1.84543700 4.69686000 -0.13812700
H -2.43240300 3.98157400 -1.65821600
O -0.17856100 -1.60801400 0.54763800
O -2.53862800 -0.75161400 0.05984200
C -2.49091100 -1.77719800 1.04830100
H -3.35703100 -2.43450600 0.85986000
C -1.19215400 -2.55842000 0.86152100

H -0.90294800 -3.02958900 1.81776400
C -2.60909300 -1.13848500 2.41958600
H -3.49682100 -0.49619500 2.45665900
H -2.69772000 -1.90419500 3.20222300
H -1.72628200 -0.51754300 2.62161700
C -1.29217500 -3.61884000 -0.21842500
H -0.30911900 -4.06785700 -0.40609100
H -1.98385000 -4.41597500 0.08591700
H -1.65734500 -3.19071100 -1.16117500
C 0.08822400 3.19228100 1.62959500
H -0.23340200 4.24220000 1.59901000
H 0.26247900 2.92140800 2.67888000
H 1.04594700 3.10873900 1.08939500
O 1.10758200 0.56423000 -1.03330400
H 1.01335300 1.49584600 -1.27554100
N 2.61593700 -0.01761000 0.90990500
C 3.77806200 0.90249900 0.88943000
C 3.01405800 -1.37400800 0.43566600
C 2.00409200 -0.08698500 2.25039500
C 4.44188600 0.88174800 -0.47513600
H 4.48829700 0.56959100 1.66218300
H 3.41644500 1.90649400 1.15062500
C 3.71448800 -1.27156000 -0.90254600
H 2.08998300 -1.96197500 0.37069800
H 3.68639200 -1.80709300 1.19277400
H 2.74756400 -0.47313000 2.96174900
H 1.12742900 -0.73879000 2.19233300
H 1.67439100 0.91365400 2.54379500
H 5.34224100 1.50665100 -0.45963600
H 3.75117300 1.28731500 -1.23600500
O 4.83977800 -0.42014500 -0.81575600
H 4.08131900 -2.25739300 -1.20747400
H 3.00714800 -0.90329100 -1.66378200
H 1.85815100 0.35802700 0.12391500

34

C -0.18832700 2.19045100 1.10318400
O 0.05043700 0.82642400 0.95658300
Os -0.93645900 -0.04367200 -0.67639500
O -1.39157000 1.85389500 -0.86171100
C -0.49033700 2.75363200 -0.28911300
C -1.11424300 4.13190000 -0.28118600
O -1.40808100 -0.59771300 -2.20595100
H -1.10656900 2.34296400 1.71379300
H 0.47617700 2.78460100 -0.84314600
H -2.03525400 4.12082000 0.31629300
H -0.42683000 4.87972800 0.13690900
H -1.37621100 4.43709300 -1.30073200
O -0.44962700 -1.67507000 0.27902700
O -2.50902600 -0.16101300 0.41324000
C -2.53695500 -1.22883900 1.34605900
H -3.56859300 -1.62322900 1.34679400
C -1.57824800 -2.32005500 0.86187800
H -1.20584000 -2.89595000 1.73013600
C -2.19464300 -0.68774200 2.72265900
H -2.88658400 0.12106100 2.98610900
H -2.26719100 -1.47294100 3.48775400
H -1.17817100 -0.27318100 2.71192300
C -2.22022900 -3.26581100 -0.13505700
H -1.47210900 -3.95431100 -0.54585800
H -3.01115500 -3.85732300 0.34563300
H -2.66838500 -2.71111300 -0.97050300

C 0.98717900 2.87922400 1.76733800
H 0.78362100 3.93966300 1.96721000
H 1.22913200 2.39894800 2.72558500
H 1.87247900 2.82170000 1.11195900
O 0.95382600 0.21369700 -1.38607500
H 0.95566900 1.04359000 -1.88519300
N 2.40351800 -0.64188300 0.89060300
C 3.58966900 0.24507500 1.05191900
C 2.73358700 -1.83573900 0.04375400
C 1.86688800 -1.06716600 2.20429000
C 4.18490000 0.55785000 -0.30481900
H 4.31722300 -0.29507600 1.67391300
H 3.25446800 1.14579600 1.58131300
C 3.45399400 -1.43447200 -1.22818800
H 1.77742000 -2.33025500 -0.16468600
H 3.37053000 -2.48082000 0.66609100
H 2.63560800 -1.65156600 2.72302500
H 0.96488400 -1.65481000 2.01381800
H 1.59800100 -0.17569100 2.77559600
H 5.07731200 1.18204300 -0.18361700
H 3.44692800 1.11243500 -0.91272100
O 4.57986000 -0.62588300 -0.94592600
H 3.82653200 -2.33598600 -1.72689900
H 2.74983500 -0.91209100 -1.89112900
H 1.64738000 -0.07838200 0.41266300

35

C 0.48081000 1.82448300 1.26405300
O 0.46263500 0.48816000 0.84726800
Os -1.12650800 0.16535600 -0.67677600
O -0.95939600 2.12712800 -0.54189700
C 0.20324200 2.66382200 0.01865400
C -0.03338100 4.13287400 0.29502500
O -2.20457900 0.04948300 -1.96950500
H -0.37585700 1.98604600 1.94976100
H 1.09037500 2.54880700 -0.64994700
H -0.82773800 4.25061900 1.04405900
H 0.87926300 4.62282500 0.66013500
H -0.35443500 4.64285200 -0.62023900
O -0.85799200 -1.64723500 -0.06237400
O -2.25980900 0.26521200 0.87351000
C -2.39039600 -0.92082800 1.63499100
H -3.46945000 -1.04627200 1.83876900
C -1.90960300 -2.10532300 0.78641000
H -1.47321500 -2.88071200 1.44279500
C -1.64980600 -0.75792500 2.94954600
H -2.03970700 0.11295300 3.49019400
H -1.76929600 -1.64466800 3.58707600
H -0.58394200 -0.58658500 2.75266500
C -3.01810000 -2.71499200 -0.04949000
H -2.61037300 -3.46608300 -0.73608800
H -3.76757500 -3.19734700 0.59226700
H -3.52543700 -1.94515200 -0.64702900
C 1.76361600 2.18210500 1.98427800
H 1.70887900 3.18640900 2.42327900
H 1.94597100 1.47213000 2.80420700
H 2.62793400 2.16140300 1.30115600
O 0.48800500 0.10526600 -1.78667900
H 0.64426600 1.01574200 -2.08780300
N 2.35970300 -1.14507600 0.63112700
C 3.68296700 -0.62614800 1.04780600
C 2.46103300 -1.89856800 -0.65269700

C 1.78689600 -2.00782900 1.68051300
C 4.33399100 0.12579700 -0.09300200
H 4.31272300 -1.48340100 1.33324100
H 3.53305400 0.01222500 1.92802200
C 3.24407600 -1.11925700 -1.68793600
H 1.43671500 -2.08827800 -0.99578800
H 2.96759800 -2.85047200 -0.42626400
H 2.45783000 -2.85529700 1.87434000
H 0.81043000 -2.35404400 1.32916000
H 1.65680700 -1.41624500 2.59385100
H 5.32219100 0.48993700 0.21065800
H 3.71051200 1.00068300 -0.36913900
O 4.50729100 -0.71875300 -1.19693200
H 3.42180300 -1.75060400 -2.56492500
H 2.65344600 -0.24508600 -1.99776800
H 1.57262700 -0.26727700 0.58038000

36

C 1.98193600 1.69784500 2.17502900
O 2.20327000 1.67358100 0.77184200
Os -0.98519100 -0.35489200 0.41313800
O 0.45329800 -0.10010400 1.85432800
C 0.59578600 1.13389200 2.50183000
C 0.38296500 0.93215600 3.99132100
O -0.66694400 1.73419400 -0.07598200
O -1.12922000 -2.24066000 0.80262700
O -2.27711300 -0.77514600 -1.03807800
H 2.72732100 1.03540700 2.67011700
H -0.14396100 1.86732200 2.12876800
H -0.60709900 0.48844800 4.15001900
H 1.13530000 0.23591100 4.39098800
H 0.43777600 1.87194800 4.55767400
C -1.92497200 -2.96136400 -0.13853000
H -2.46549400 -3.73338800 0.43670300
C -2.92729400 -2.01264300 -0.79634300
H -3.22452500 -2.42485800 -1.77807300
C -4.17333400 -1.80792900 0.04989700
H -4.74994200 -2.74034800 0.12440600
H -3.91275000 -1.48044200 1.06439300
H -4.81663800 -1.04203400 -0.40287000
C -1.02476700 -3.63386600 -1.15951500
H -0.27572400 -4.25978500 -0.65483000
H -1.60608000 -4.28024000 -1.83102600
H -0.51119400 -2.87441000 -1.76651900
C 2.18153300 3.12157500 2.64478200
H 2.15717400 3.20129400 3.73865900
H 3.14634800 3.50688400 2.29253200
H 1.38972900 3.76169900 2.22650700
O 0.45950300 -0.55538600 -0.69516700
H 1.53503500 1.06288000 0.40602100
H 1.47783600 -1.18826300 -0.22996500
C 0.56913400 3.82971700 -1.44547600
C -0.90060300 3.77081600 -1.08841500
C -1.04458500 1.73294400 -2.44206800
C 0.42480500 1.91845800 -2.74592000
H -1.10029700 4.14333400 -0.07783300
H 1.16276700 3.30217300 -0.67999000
H 0.88736900 4.87807500 -1.48519500
H -1.34582200 0.68033300 -2.39075700
H -1.66511500 2.26742400 -3.17484900
H 1.01973200 1.33491500 -2.02718700
H 0.62976500 1.54442600 -3.75592300
H -1.50725200 4.31505400 -1.82473300

O 0.77938300 3.28307000 -2.72783800
C -2.83511200 2.27788200 -0.83986300
H -3.35306600 2.87839700 -1.59595500
H -3.13513800 1.22572000 -0.89567700
H -3.00168700 2.67275200 0.16568800
O -2.14864800 0.27825000 1.50322600
N -1.36893800 2.33951600 -1.09510000
N 2.41125700 -1.89438200 0.09209600
C 2.62369400 -2.81947000 -1.04318900
C 3.62280700 -1.06612700 0.29918700
C 2.03492300 -2.61242800 1.32313100
C 3.03933700 -2.03708400 -2.27298500
H 1.68531600 -3.36190500 -1.21228400
H 3.41012200 -3.53864300 -0.76173500
C 4.01091100 -0.37648000 -0.99111100
H 3.39845700 -0.32541700 1.07400700
H 4.43195800 -1.73309300 0.63964900
H 1.82094800 -1.86708000 2.09641600
H 1.10697700 -3.16414200 1.13883200
H 2.84892400 -3.29038600 1.61733800
H 2.21601400 -1.36141600 -2.57175100
H 3.24558800 -2.72226400 -3.10302500
O 4.21692800 -1.30805400 -2.02999700
H 3.23327700 0.35369400 -1.27280700
H 4.94967300 0.17052500 -0.85345000

37

C 0.38558700 -3.09023500 -0.97411500
O -0.22022200 -2.88863100 0.29004900
Os -0.17148700 0.85078700 -0.33804300
O 1.11392300 -0.77586900 -0.87105300
C 0.60455400 -1.76779600 -1.72366900
C 1.53459300 -1.94016300 -2.91391100
O -1.83547600 -0.68834400 -0.36366900
O 1.29615100 2.10631100 -0.29126500
O -1.25671000 2.42879100 0.18288500
H 1.38179600 -3.53777100 -0.77145800
H -0.37944300 -1.44678000 -2.11023900
H 1.70688700 -0.95864100 -3.37131300
H 2.50736900 -2.34933100 -2.59593000
H 1.12040500 -2.61038600 -3.67901300
C 0.93254500 3.37796100 0.25033100
H 1.55312300 4.12658100 -0.27279900
C -0.54316300 3.63600000 -0.04363700
H -0.93199900 4.38098100 0.67497200
C -0.77704700 4.13661100 -1.45861800
H -0.31974300 5.12482900 -1.60737700
H -0.35318800 3.43826300 -2.19110300
H -1.85414500 4.22249100 -1.65386100
C 1.24095300 3.41043300 1.73617000
H 2.29070400 3.14031300 1.91648700
H 1.07333600 4.41347000 2.15196000
H 0.59777700 2.69945900 2.27183700
C -0.43556000 -4.08026500 -1.78120700
H 0.07171200 -4.39378500 -2.70271300
H -0.64450700 -4.97306200 -1.17962200
H -1.39769800 -3.62251100 -2.05772900
O -0.01192800 0.23388600 1.29974800
H -0.73799600 -2.05909000 0.24299400
H 1.84430500 -1.14528200 0.44490600
C -3.62371000 -2.55810800 0.86154900
C -3.98784000 -1.51146500 -0.17086600

C -3.18702700 0.18791600 1.39992000
C -2.84291400 -0.94683400 2.33583800
H -3.84311300 -1.86587300 -1.19708900
H -2.61255800 -2.95483100 0.67272200
H -4.33686800 -3.38801100 0.78949200
H -2.50070500 1.03839600 1.47898800
H -4.22148800 0.52254300 1.55936500
H -1.79769100 -1.25508100 2.17685100
H -2.95088500 -0.60558300 3.37145900
H -5.02434000 -1.17774600 -0.02833300
O -3.73265400 -2.03012800 2.16134400
C -3.58062100 0.76940000 -0.96257300
H -4.64105400 0.96696800 -0.76916600
H -2.97017700 1.66135700 -0.78125200
H -3.41868500 0.39598700 -1.97664300
O -0.58409400 0.91542100 -2.01859400
N -3.11159400 -0.29700200 -0.02970700
N 2.53420200 -1.30727100 1.27747300
C 3.63519500 -2.16671300 0.76440500
C 3.06210700 0.03043600 1.68862400
C 1.80907000 -1.96176700 2.38704100
C 4.43515200 -1.42910900 -0.29302100
H 3.17964500 -3.08343100 0.36542300
H 4.27538000 -2.42656000 1.62038800
C 3.88248200 0.63225500 0.56848500
H 2.19169800 0.65037800 1.93427000
H 3.68217600 -0.13339600 2.58302900
H 1.00698500 -1.28791500 2.69886700
H 1.36219300 -2.88792100 2.01439400
H 2.51416200 -2.15150500 3.20609200
H 3.79597800 -1.23127700 -1.17148100
H 5.28443400 -2.04686700 -0.60759200
O 4.94936900 -0.22817100 0.22012300
H 3.23628700 0.84453500 -0.29821900
H 4.32171200 1.57869500 0.90434900

38

C 0.48423800 -3.18207600 -0.50745900
O -0.18173700 -2.86217600 0.69671900
Os -0.22828000 0.80574900 -0.28962300
O 1.10804900 -0.86720900 -0.72903900
C 0.59920800 -1.97304800 -1.43999900
C 1.47174400 -2.26095000 -2.64855000
O -1.85262300 -0.68229800 -0.39490800
O 1.23304300 2.08225500 -0.16805200
O -1.34050300 2.36304000 0.14568500
H 1.52518500 -3.50628700 -0.26613600
H -0.41767400 -1.72968300 -1.79061900
H 1.61683600 -1.32985800 -3.20915400
H 2.46103000 -2.64089400 -2.34506400
H 1.02032600 -3.00253500 -3.32109300
C 0.82523100 3.35679500 0.32436900
H 1.45665600 4.10720200 -0.18398600
C -0.63633500 3.58653600 -0.04865800
H -1.08251200 4.32253100 0.64391000
C -0.81040900 4.06837600 -1.47763300
H -0.34403600 3.36728500 -2.18136400
H -1.87789500 4.14129000 -1.72475600
H -0.35738600 5.05979400 -1.61595500
C 1.05950100 3.43106400 1.82231400
H 2.11388300 3.23067800 2.05609300
H 0.81180000 4.42772600 2.21250600

H 0.43923600 2.68744400 2.34052500
C -0.24514800 -4.34828600 -1.14059700
H 0.31436000 -4.78209900 -1.97865800
H -0.41176100 -5.13292800 -0.39274700
H -1.22757100 -4.01544400 -1.50851100
O -0.08295700 0.14882100 1.33946700
H -0.21948600 -1.88922300 0.78471100
H 2.00905600 -1.05796100 0.31522000
C -3.63907900 -2.52821300 0.72555500
C -3.96434700 -1.56712000 -0.39837900
C -3.42405700 0.25876200 1.14133000
C -3.14664300 -0.79739000 2.18632100
H -3.69284300 -1.96549300 -1.38210000
H -2.57851200 -2.82640000 0.67368500
H -4.26761400 -3.42129200 0.62792900
H -2.78514400 1.14308600 1.24002400
H -4.48220400 0.55498600 1.15869500
H -2.07484800 -1.04742900 2.18812000
H -3.41333100 -0.40138700 3.17289100
H -5.02613700 -1.28603700 -0.38023400
O -3.94432900 -1.94167000 1.97063200
C -3.55904200 0.68668000 -1.27976600
H -4.63920600 0.86044900 -1.21517000
H -2.99772400 1.60733200 -1.08984700
H -3.27854100 0.26194200 -2.24677200
O -0.46154800 0.82823300 -2.00241400
N -3.16366800 -0.30292600 -0.23779500
N 2.80783100 -1.12507200 1.15056700
C 3.93745600 -1.93233800 0.62837300
C 3.25433700 0.26595600 1.44076900
C 2.19677700 -1.74108900 2.34316200
C 4.58466000 -1.21731400 -0.54158100
H 3.54139800 -2.91439200 0.33451400
H 4.66462000 -2.07057300 1.44371600
C 3.94489800 0.85302900 0.22880400
H 2.35860800 0.84042800 1.70275600
H 3.94240200 0.21809000 2.29984200
H 2.95351800 -1.83163900 3.13394900
H 1.36727600 -1.10140600 2.66189300
H 1.79060600 -2.72212000 2.07583900
H 3.85281500 -1.12752600 -1.36518900
H 5.44784400 -1.79127700 -0.89786600
O 5.04459100 0.05075900 -0.15489500
H 3.22168600 0.95840700 -0.59489800
H 4.33157100 1.85000800 0.46942400

11ts

O 0.90468600 0.63171800 -1.07025100
O 0.68617600 -0.53654400 1.16440300
C 2.15266000 0.55158200 -0.37096800
C 2.04455000 -0.54657100 0.67375500
H 2.91184000 0.28984800 -1.12575000
C 2.36334200 -1.92606300 0.14114100
H 2.67303800 -0.31419600 1.54752500
H 2.13735800 -2.69039700 0.89287600
H 1.77101000 -2.14258800 -0.75987100
H 3.42522800 -2.00194100 -0.12581300
Os -0.60105700 -0.04909900 -0.13850100
C 2.43812700 1.91686700 0.21993900
H 3.44040800 1.95040100 0.66631600
H 2.36867000 2.68671600 -0.55569700
H 1.69798000 2.15196900 0.99727400
O -1.29140800 1.61836300 0.02077900

H -2.10597500 1.06371900 0.86844400
O -2.19869400 -0.05306100 1.24096300
H -1.87829000 -0.15616800 2.15203700
O -1.19488500 -1.29556400 -1.10770700

11TS_2

O 1.12404400 0.63426100 -1.10496600
O 0.81667400 -0.34685500 1.24341800
C 2.24097100 0.86994700 -0.24889500
C 2.20328000 -0.13519600 0.89596000
H 3.14517200 0.70420800 -0.85822400
C 2.83363000 -1.46591400 0.54912400
H 2.66871100 0.28850200 1.79981600
H 2.65258300 -2.19855600 1.34377300
H 2.41690800 -1.86087200 -0.38852800
H 3.91780000 -1.35595900 0.41729200
Os -0.35481500 -0.22072200 -0.23923400
C 2.18802600 2.30948100 0.22379800
H 3.09578000 2.57294300 0.78286800
H 2.09186300 2.98373200 -0.63379400
H 1.31807200 2.46631000 0.87608000
O -1.25841300 1.33009500 -0.40383100
H -2.78744900 0.09542900 1.04940900
O -1.88606500 -0.76906400 1.06005000
H -1.48647200 -0.91742900 1.93144500
O -0.50271200 -1.62927600 -1.16253700
O -3.34065600 1.07066800 0.75164100
H -4.06021200 0.85060000 0.14130500
H -2.42526700 1.35745600 0.13019600

7. References:

1. Criegee, R.; Marchand, B.; Wannowius, H. Zur Kenntnis der organischen Osmium-Verbindungen. II. Mitteilung. *Leibigs Ann. Chem.* **1942**, *550*, 99-133.