Uranyl Extraction by *N,N*-Dialkylamide Ligands Studied by Static and Dynamic DFT Simulations

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- Supporting Information -

Full reference 25:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S1: Atomic coordinates (in Å) and RESP atomic charges (in e) on **L**, as obtained from B3LYP/6-31G** calculations:

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TYPE	X(Å)	Y(Å)	Z(Å)	Q(e)
H	2.756	1.480	-0.588	0.0181
N	4.706	-0.689	1.039	-0.1199
H	3.548	-1.932	2.293	0.0481
C	3.752	1.054	-0.444	-0.0015
H	4.157	0.779	-1.427	0.0181
H	5.247	-1.686	2.804	0.0481
H	4.414	1.800	0.008	0.0181
H	4.872	-2.768	1.433	0.0481
O	2.503	-0.748	0.575	-0.5107
C	4.579	-1.843	1.948	-0.0266
C	3.617	-0.182	0.419	0.3912
C	6.083	-0.220	0.831	-0.0805
H	6.467	0.245	1.751	0.0498
H	6.140	0.495	0.011	0.0498
H	6.720	-1.083	0.590	0.0498

Table S2: Reaction free energies (ΔG, in kcal/mol) according to eq. 4 (see Text) using different density functionals to compute the ΔE_{gas} term. All other energy components are the same as in Table 1 (see Text).

	ΔG (kcal/mol) in SMD-water		
	BLYP-D3	**PBE0-D3**	**M06-2X**
0.5.0 + **L** → **0.4.1** + H_2O	-9.2	-4.9	-3.3
0.5.0 + 2 **L** → **0.3.2a** + 2 H_2O	-16.1	-10.1	-7.8
0.5.0 + 2 **L** → **0.3.2b** + 2 H_2O	-16.7	-10.4	-8.4
0.5.0 + NO_3^- → **1.4.0a** + H_2O	-2.5	-1.1	0.2
0.5.0 + NO_3^- → **1.4.0b** + H_2O	-6.1	-1.9	1.5
0.5.0 + NO_3^- → **1.3.0…H_2O** + H_2O	-9.4	-7.6	-3.2
0.5.0 + NO_3^- → **1.3.0** + 2 H_2O	-11.7	-8.9	-4.6
0.5.0 + **L** + NO_3^- → **1.2.1** + 3 H_2O	-18.7	-14.2	-9.5
0.5.0 + 2 **L** + NO_3^- → **1.1.2a** + 4 H_2O	-24.2	-19.1	-14.8
0.5.0 + 2 **L** + NO_3^- → **1.1.2b** + 4 H_2O	-24.6	-19.0	-13.9
0.5.0 + 2 **L** + NO_3^- → **1.2.2a** + 3 H_2O	-16.4	-10.8	-8.4
0.5.0 + 2 **L** + NO_3^- → **1.2.2b** + 3 H_2O	-16.7	-10.1	-9.1
0.5.0 + 2 **L** + NO_3^- → **1.2.2c** + 3 H_2O	-17.2	-11.0	-8.0
0.5.0 + 2 **L** + NO_3^- → **1.2.2d** + 3 H_2O	-15.2	-9.3	-6.1
0.5.0 + 2 NO_3^- → **2.2.0** + 3 H_2O	-11.9	-11.5	-8.6
0.5.0 + **L** + 2 NO_3^- → **2.1.1** + 4 H_2O	-16.8	-14.9	-12.1
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2a** + 5 H_2O	-20.0	-16.6	-13.1
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2b** + 5 H_2O	-23.7	-18.1	-15.3
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2c** + 5 H_2O	-23.3	-16.8	-12.5
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2d** + 5 H_2O	-21.1	-18.1	-16.6
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2e** + 5 H_2O	-21.2	-12.4	-6.4
0.5.0 + 2 **L** + 2 NO_3^- → **2.0.2f** + 5 H_2O	-22.7	-13.5	-8.0
0.5.0 + 2 **L** + 2 NO_3^- → **$TS_{2.0.2a-2.0.2b}$** + 5 H_2O	-19.0	-15.0	-12.0
0.5.0 + 2 **L** + 2 NO_3^- → **$TS_{2.0.2b-2.0.2c}$** + 5 H_2O	-22.2	-13.9	-9.3
0.5.0 + **L** + 2 NO_3^- → **2.0.1** + 5 H_2O	-22.7	-18.6	-11.2
0.5.0 + 2 **L** + 2 NO_3^- → **2.1.2a** + 4 H_2O	-16.8	-12.1	-9.6
0.5.0 + 2 **L** + 2 NO_3^- → **2.1.2b** + 4 H_2O	-13.0	-6.3	-7.8
0.5.0 + 2 **L** + 2 NO_3^- → **2.1.2c** + 4 H_2O	-18.1	-12.7	-11.1
0.5.0 + 2 **L** + 2 NO_3^- → **2.1.2d** + 4 H_2O	-9.1	-4.8	-3.2
0.5.0 + 2 **L** + 2 NO_3^- → **1.1.2a…NO_3^-** + 4 H_2O	-14.4	-8.9	-6.8
0.5.0 + 2 **L** + NO_3^- → **2.0.2b…H_2O** + 4 H_2O	-17.9	-11.7	-8.1
0.5.0 + 2 **L** + 2 NO_3^- → **$TS_{1.1.2a...NO3-2.1.2d}$** + 4 H_2O	-9.7	-5.3	-3.6
0.5.0 + 2 **L** + 2 NO_3^- → **$TS_{2.1.2d-2.0.2b}$** + 4 H_2O	-10.6	-5.2	-2.7
0.5.0 + 2 NO_3^- → **2.3.0a** + 2 H_2O	-4.8	-1.3	1.9
0.5.0 + **L** + 2 NO_3^- → **2.2.1** + 3 H_2O	-15.5	-11.1	-8.0
0.5.0 + **L** + 2 NO_3^- → **2.0.1** + 5 H_2O	-22.7	-18.6	-11.2
0.5.0 + 2 **L** + NO_3^- → **1.0.2** + 5 H_2O	-26.5	-19.4	-10.8

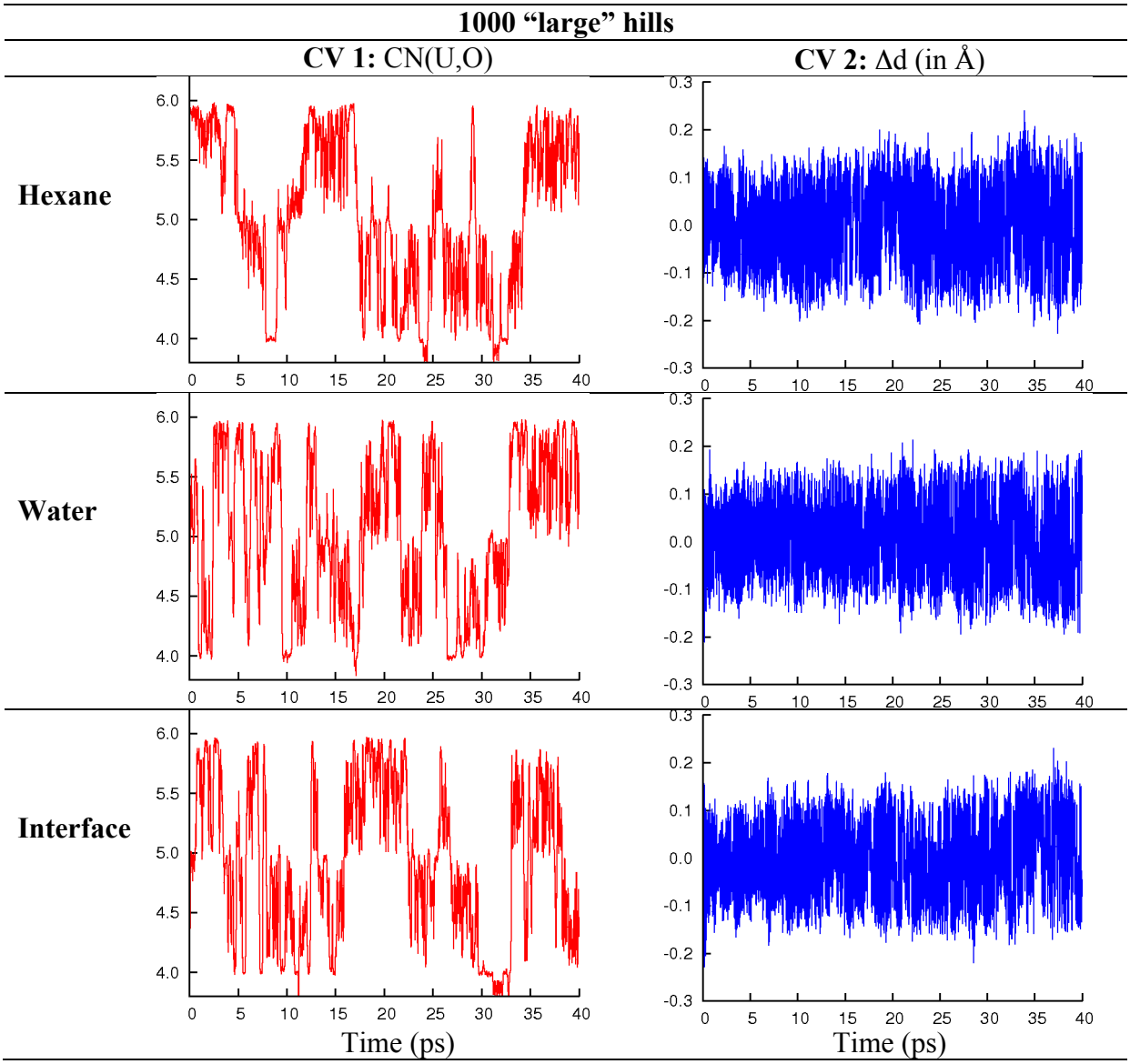

Figure S1: Time evolution of the two collective variables (CVs) during DFT/MM-MD simulations of **2.0.2a-c** in the three solvent environments over 40 ps (1000 hills). The resulting free energy surfaces are given in Figure 2 (see Text). "Large" hills are defined as: WW = 0.5 kcal/mol, CV1: 0.05, CV2: 0.02 Å.

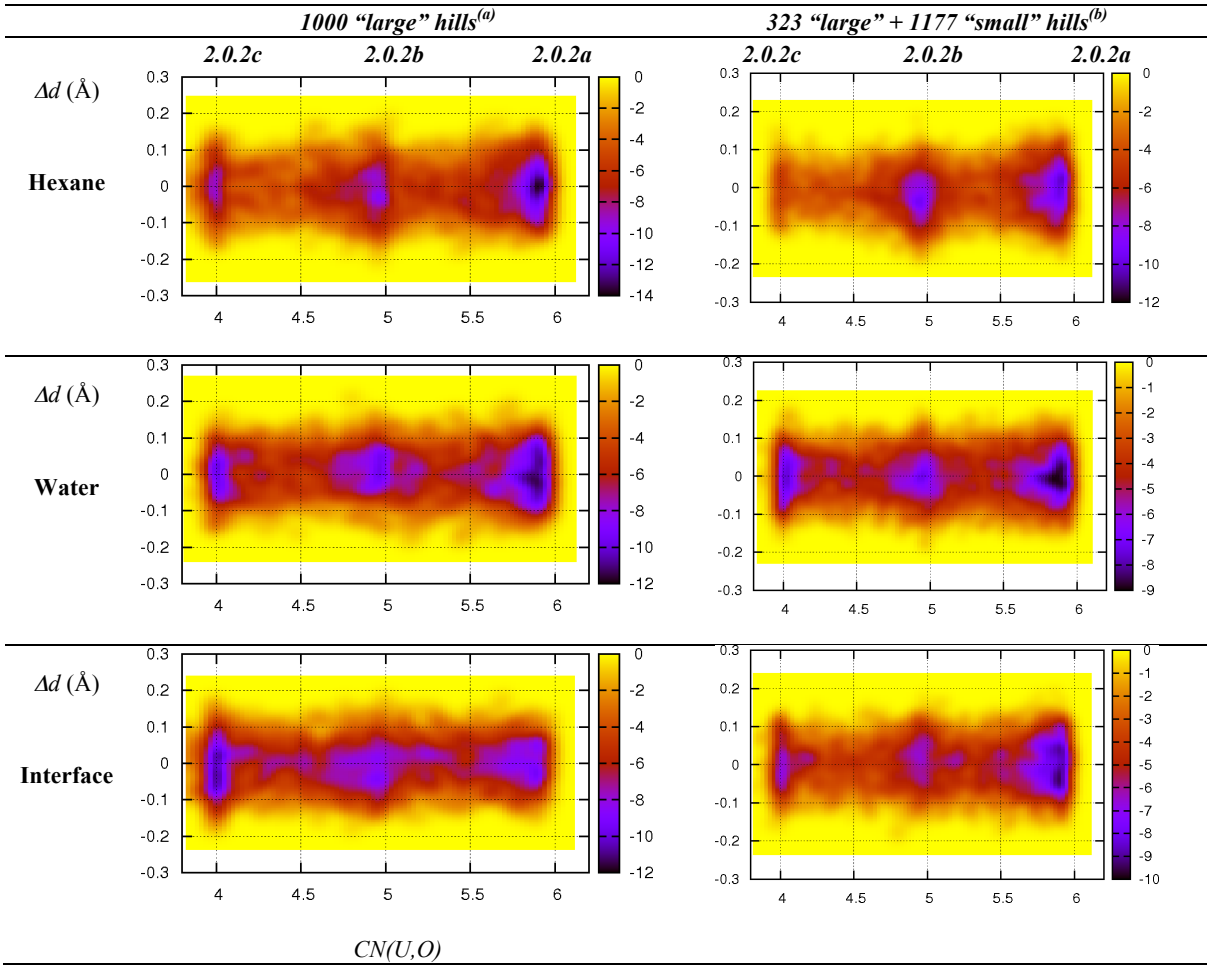

Figure S2: Free energy surfaces (colour coded in kcal/mol) of **2.0.2a-c** as obtained from DFT/MM metadynamics simulations in hexane, water and at the interface. *X-axis*: Equatorial coordination number around uranyl. *Y-axis*: differences between the two U-N_{nit} distances (in Å). Comparison of two sets of sampling parameters.
a 1000 "large" hills (height: 0.5 kcal/mol, scale factors: CV1: 0.05, CV2: 0.02 Å).
b 323 "large" hills (height: 0.5 kcal/mol, scale factors: CV1 0.05; CV2 0.02 Å) followed by 1177 "small" hills (height: 0.25 kcal/mol, scale factors: CV1: 0.04; CV2: 0.016 Å).

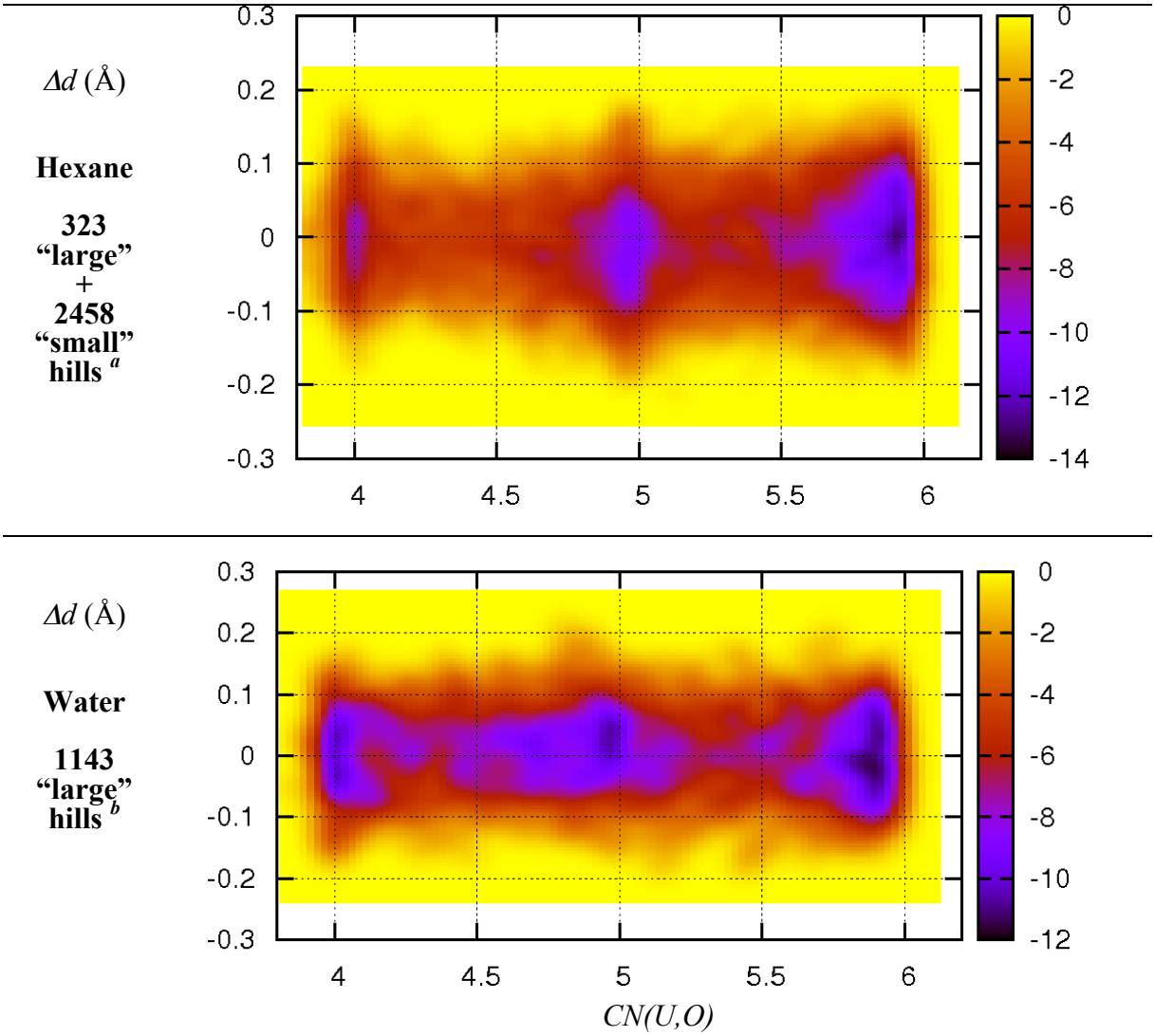

Figure S3: Extension of selected metadynamics simulations. Free energy surfaces (colour coded in kcal/mol) of **2.0.2a-c** as obtained from DFT/MM metadynamics simulations in hexane (*top*) and in water (*bottom*) using different sampling parameters compared to Figure 3. *X-axis*: Equatorial coordination number around uranyl. *Y-axis*: differences between the two U-N_{nit} distances (in Å).
a 323 "large" hills (height: 0.5 kcal/mol, scale factors: CV1 0.05; CV2 0.02 Å) followed by 2458 "small" hills (height: 0.25 kcal/mol, scale factors: CV1: 0.04; CV2: 0.016 Å).
b 1143 "large" hills (height: 0.5 kcal/mol, scale factors: CV1: 0.05, CV2: 0.02 Å).

XYZ Coordinates in Å (BLYP-D3/SDD optimized geometries with G09).

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Complex 0.5.0

U	0.012735	-0.035335	0.000147
O	0.038903	-0.060786	1.784047
O	0.047288	-0.125680	-1.781432
O	-2.442698	0.076026	-0.450023
O	-0.766366	2.295186	0.511510
O	-0.828905	-2.361484	0.206633
O	1.933134	1.505522	-0.393308
O	2.043866	-1.453590	0.122359
H	-3.187238	0.197338	0.174978
H	-2.828663	-0.013958	-1.346210
H	-0.859635	2.632911	1.426595
H	-1.025813	3.020731	-0.093373
H	-0.937693	-2.844188	1.052540
H	-1.106791	-2.968656	-0.510436
H	2.439936	2.041612	0.251293
H	2.324855	1.668669	-1.276600
H	2.456595	-1.786066	0.946679
H	2.581348	-1.788220	-0.625513

30
Complex 0.4.1

U	0.378976	0.273896	-0.269092
O	2.662638	1.327037	-0.552891
O	-1.452992	-0.544603	-1.836791
O	0.602169	1.066265	-2.712929
O	1.277510	-1.254315	-0.543996
O	-0.303914	1.915491	-0.013595
O	1.362646	0.365402	2.033510
H	3.495528	0.813141	-0.551179
H	2.902746	2.260074	-0.381953
H	-1.786833	-1.462366	-1.785689
H	-1.358303	-0.327867	-2.787118
H	1.321575	0.770634	-3.307970
H	0.447109	2.011409	-2.918523
H	1.213261	1.062471	2.703204
H	1.906032	-0.330460	2.454809
O	-1.280308	-0.705362	0.941782
C	-2.453337	-0.616229	1.511863
C	-3.242105	0.671775	1.412483
H	-3.630872	0.986336	2.392270
H	-4.104508	0.541633	0.737124
H	-2.600661	1.462219	1.006329
N	-2.937268	-1.675269	2.165133
C	-2.163763	-2.936751	2.311355
H	-2.075955	-3.173703	3.382146
H	-2.708253	-3.751382	1.810431
H	-1.170042	-2.824510	1.868544
C	-4.266358	-1.649615	2.840137
H	-4.612811	-2.683910	2.954298
H	-4.174540	-1.191143	3.837311
H	-5.001254	-1.096751	2.243204

42
Complex 0.3.2a

U	0.776011	-0.308448	-0.625571
O	1.656359	-0.082197	0.933686
O	0.106502	-0.441438	-2.292263
O	-1.380353	-1.443001	0.223954
O	-0.846808	1.235786	0.031460
N	-2.135223	3.070281	0.405454
C	-2.862023	2.872121	-0.875061
C	-0.363040	2.501264	2.058922
C	-2.577572	4.244285	1.201562
H	-3.887152	2.528649	-0.665824
H	-2.913533	3.836042	-1.401887
H	0.020304	3.531426	2.108625
H	-2.339872	2.136455	-1.494129
H	0.476432	1.798385	2.106481
H	-1.003502	2.338876	2.941282
H	-2.153286	5.166219	0.773378
H	-3.673841	4.302441	1.152164
H	-2.280149	4.154666	2.250751
C	-1.139990	2.255980	0.779292
O	1.697708	1.969397	-1.307224
H	1.818146	-2.454960	2.346020
N	1.805827	-4.680532	0.182629
H	1.510050	-4.301496	-1.888298
C	1.030143	-3.136637	1.985606
H	0.963428	-4.000298	2.655227
H	1.537146	-6.032694	-1.416334
H	0.083091	-2.579989	2.018605
H	3.066187	-5.104300	-1.474712
O	1.054017	-2.604469	-0.378634
C	1.990744	-5.045471	-1.246164
C	1.311061	-3.490475	0.540599
C	2.183518	-5.733120	1.169228
H	2.677805	-5.294166	2.043819
H	2.889155	-6.417242	0.682245
H	1.295196	-6.303013	1.482433
O	3.004891	-0.696207	-1.790441
H	3.845975	-0.956333	-1.366430
H	3.040941	-1.010774	-2.715569
H	-2.162721	-0.855604	0.204250
H	-1.638510	-2.267387	-0.235270
H	1.702528	2.260586	-2.240835
H	2.493919	2.355481	-0.891586

42
Complex 0.3.2b

U	-0.520812	0.321794	-0.148158
O	-0.306307	0.930223	-1.829015
O	-0.999853	-0.231549	1.497990
O	-2.302060	-1.207747	-1.144170
O	1.637026	0.983278	0.398276
N	3.868843	1.267793	0.144880
C	4.100600	0.180633	1.131018
C	2.320983	2.786362	-1.095240
C	5.082772	1.864995	-0.471271
H	3.971422	-0.802225	0.650432
H	5.125327	0.266930	1.511951
H	3.041831	3.608730	-1.003083
H	3.391941	0.274475	1.962766
H	1.314490	3.163043	-0.879545
H	2.328029	2.424516	-2.136956
H	5.576704	2.536030	0.248574
H	5.773410	1.051389	-0.734572
H	4.836216	2.416083	-1.383593
C	2.617883	1.637991	-0.152769
O	-0.510882	2.726152	0.796940
H	1.272072	-4.359530	-1.912138
N	1.785735	-3.202083	0.665419
H	1.617117	-1.463061	1.885170
C	1.715001	-3.353743	-1.832068
H	2.803813	-3.455287	-1.959237
H	1.924313	-2.998045	2.762013
H	1.321134	-2.726019	-2.639937
H	0.298343	-2.642595	2.093671
O	0.633055	-1.641341	-0.519723
C	1.380249	-2.533527	1.932153
C	1.364095	-2.705218	-0.505942
C	2.581237	-4.448437	0.802608
H	2.799138	-4.894716	-0.171645
H	2.013419	-5.171623	1.407621
H	3.528134	-4.221098	1.315088
O	-2.794172	1.581916	-0.212244
H	-3.180560	1.824024	-1.078449
H	-3.539841	1.271031	0.340159
H	-2.312904	-1.402709	-2.102573
H	-2.687488	-1.985685	-0.694457
H	-0.024838	2.908183	1.625293
H	-1.390672	3.146879	0.883586

19
Complex 1.4.0a

U	-0.418198	-0.011734	0.137675
O	-2.720902	-2.620278	2.395885
O	-1.988048	-1.876344	0.418164
O	-1.755844	1.184914	0.065757
O	-1.571732	-0.987381	-2.034813
O	1.140974	2.051495	0.023262
O	-1.287602	-0.909697	2.249215
O	0.974133	-1.146505	0.154940
O	0.661139	0.870176	2.387489
O	0.491954	0.727428	-2.170470
N	-2.048859	-1.858764	1.736779
H	-2.491115	-0.650590	-2.081895
H	1.370477	2.371202	0.920677
H	0.788148	2.816969	-0.473108
H	-1.667634	-1.962930	-2.004054
H	1.461956	0.664112	-2.279452
H	1.280196	0.190231	2.727111
H	0.086322	0.205545	-2.893882
H	0.000554	0.982156	3.103657

19
Complex 1.4.0b

U	0.187175	0.284182	-0.576629
O	2.449720	1.359298	-0.100708
O	-2.212824	-2.948122	0.435828
O	-1.444743	-0.403086	-2.418706
O	-1.554276	-0.812155	0.331527
O	1.116963	0.931398	-2.855082
O	1.106295	-1.254177	-0.720616
O	-0.825507	-2.160139	1.982811
O	-0.519545	1.936808	-0.454794
O	0.561926	0.193329	1.901782
N	-1.530849	-2.077676	0.949245
H	3.129438	0.770393	0.285714
H	2.506709	2.202014	0.392320
H	-2.186653	-0.923201	-2.045035
H	-1.827692	0.216497	-3.069800
H	1.689446	0.313804	-3.352034
H	1.376390	1.835946	-3.118315
H	0.104441	0.866965	2.444990
H	0.146721	-0.684455	2.162559

19
Complex 1.3.0…H_2O

U	-0.499140	0.114716	0.007316
O	3.229083	-1.668197	-0.211617
O	0.998524	-1.795529	-0.311944
O	-0.847104	-0.314253	1.718035
O	-1.784979	-1.945461	-0.684439
O	0.214024	2.303426	0.707455
O	1.942898	0.115544	0.207627
O	-0.360144	0.597718	-1.719855
O	2.436542	2.870399	-0.397628
O	-2.789264	1.124506	-0.041538
N	2.134000	-1.160623	-0.112841
H	-1.814402	-2.696901	-0.057216
H	1.076582	2.649234	0.231415
H	0.303305	2.516722	1.657638
H	-1.616597	-2.335367	-1.566664
H	-3.182923	1.611659	-0.791765
H	2.864304	1.986866	-0.383149
H	-3.418616	1.169529	0.704700
H	2.458018	3.168644	-1.327885

16
Complex 1.3.0

U	-0.035146	-0.468263	-0.101280
O	0.031286	-0.513597	1.693629
O	-0.080022	-0.672268	-1.885828
O	0.177252	-2.960714	0.003361
O	-2.493003	-0.972913	-0.003313
O	-1.312335	1.584469	-0.152844
N	-0.282706	2.415808	-0.221301
O	-0.386009	3.618938	-0.271254
O	0.873892	1.769039	-0.228388
O	2.473248	-0.553465	-0.176803
H	0.250745	-3.499745	0.815564
H	0.201354	-3.570438	-0.760369
H	2.984656	-0.188510	0.574525
H	2.934411	-0.259123	-0.989154
H	-3.004995	-0.694880	0.783957
H	-3.052243	-0.764355	-0.779837

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Complex 1.2.1

U	-0.106758	-0.518809	-0.158824
O	-0.080836	-0.421101	1.643893
O	0.041856	-0.814386	-1.931691
O	0.241027	-3.001046	0.061254
O	-2.375269	-0.929313	-0.120226
N	-4.285069	0.290887	-0.149663
C	-4.073533	0.593610	-1.591072
C	-3.548085	-0.757380	1.997743
C	-5.460998	0.937688	0.473254
H	-3.465357	1.505089	-1.684949
H	-3.550097	-0.240243	-2.071068
H	-2.697961	-1.374769	2.308671
H	-5.053270	0.743531	-2.062239
H	-4.487268	-1.291614	2.207794
H	-3.536067	0.169725	2.591909
H	-5.401490	2.023895	0.304465
H	-6.379844	0.553501	0.004068
H	-5.501900	0.747516	1.549481
C	-3.396449	-0.452533	0.519038
O	-1.259479	1.628553	-0.389060
N	-0.179319	2.392726	-0.425707
O	-0.218359	3.600962	-0.540696
O	0.935607	1.698556	-0.324817
O	2.439716	-0.622940	-0.067155
H	0.441407	-3.496607	0.878392
H	0.401391	-3.598193	-0.694932
H	2.840332	-0.080432	0.642989
H	2.898058	-0.356530	-0.890352

40
Complex 1.1.2a

U	-0.050878	-0.502045	0.090693
O	-0.090113	-0.712644	1.890649
O	-0.009837	-0.468731	-1.714366
O	0.323573	-2.993602	-0.199377
O	-2.302529	-1.192632	0.047773
N	-4.272111	-0.077155	0.195183
C	-4.116188	0.390388	-1.206777
C	-3.405888	-1.277238	2.208883
C	-5.439248	0.464876	0.921593
H	-3.556665	1.337544	-1.212931
H	-3.562800	-0.356791	-1.785425
H	-2.515833	-1.874082	2.436152
H	-5.114301	0.538625	-1.639081
H	-4.311581	-1.872529	2.401111
H	-3.413027	-0.405890	2.882022
H	-5.386741	1.565098	0.918715
H	-6.364318	0.151456	0.413690
H	-5.466904	0.114186	1.957206
C	-3.318362	-0.834697	0.758027
O	-1.495717	1.496859	0.267547
N	-0.528794	2.387640	0.371076
O	-0.730907	3.582827	0.496296
O	0.671852	1.852872	0.326336
H	2.137133	0.258907	2.598125
N	4.436927	0.371914	0.172441
H	3.858322	-0.822102	-1.476560
C	2.993380	0.782763	2.156539
H	2.720865	1.846526	2.059739
H	5.618602	-0.822055	-1.113086

H	3.863529	0.694525	2.820401
H	4.860750	0.605109	-1.891994
O	2.308615	-0.426249	0.161241
C	4.707129	-0.207030	-1.164399
C	3.244221	0.208481	0.774592
C	5.555729	1.117208	0.796469
H	6.149065	0.459427	1.452303
H	5.187188	1.975383	1.371072
H	6.205619	1.495209	-0.003491
H	0.126429	-3.676128	0.470001
H	0.181394	-3.397261	-1.077385

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Complex 1.1.2b

U	-0.054280	-0.115291	0.660619
O	-0.615818	-0.875590	-0.881012
O	0.378249	0.647038	2.244238
O	2.996424	-2.904779	1.062874
O	0.880968	-2.281186	1.420336
O	2.244057	-0.924122	0.355555
N	2.098032	-2.091858	0.953935
O	-1.961859	1.257951	0.507232
N	-4.085201	1.037620	-0.235333
C	-4.461624	0.565287	1.124449
C	-2.320548	1.837698	-1.823392
C	-5.157431	1.083685	-1.252078
H	-4.193137	1.325802	1.871153
H	-5.543833	0.392518	1.146509
H	-2.334719	0.999957	-2.538827
H	-3.926409	-0.365380	1.362707
H	-1.282873	2.174873	-1.715328
H	-2.933766	2.657297	-2.225063
H	-5.616165	0.086855	-1.340368
H	-5.929848	1.806401	-0.945788
H	-4.763469	1.373281	-2.230758
C	-2.804223	1.362595	-0.465262
O	-1.735400	-1.581158	1.985759
H	1.331384	4.663805	0.732402
N	3.038261	2.650313	-0.178119
H	3.949172	0.744724	-0.457573
C	1.046633	3.631086	0.977536
H	1.297972	3.430133	2.031466
H	4.536279	2.060411	-1.539877
H	-0.037089	3.508627	0.863562
H	2.931273	1.299945	-1.813402
O	1.011750	1.656485	-0.423959
C	3.655298	1.619307	-1.055848
C	1.726422	2.605814	0.087812
C	3.972193	3.631061	0.416644
H	3.488306	4.220867	1.200896
H	4.355506	4.305314	-0.365471
H	4.818261	3.086112	0.861902
H	-1.606313	-2.532993	1.790284
H	-1.570213	-1.495869	2.947158

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Complex 1.2.2a

U	-0.082820	-0.168586	0.561713
O	-0.109770	0.164847	-1.216130
O	-0.092704	-0.453989	2.345581
O	-1.371081	-2.457658	0.387424
O	1.294476	-2.096069	0.088736
N	3.568806	-2.136164	0.021409
C	3.621549	-2.095209	1.503325
C	2.299891	-1.979641	-2.118527
C	4.868829	-1.967325	-0.663514
H	2.723731	-2.563655	1.919095
H	4.517295	-2.632657	1.840676
H	2.734108	-1.022329	-2.446252
H	3.664723	-1.045373	1.830872
H	1.242275	-1.998186	-2.404105
H	2.834016	-2.798586	-2.623196
H	5.232029	-0.942930	-0.490956
H	5.586352	-2.692811	-0.254453
H	4.775913	-2.131404	-1.740885
C	2.386896	-2.081886	-0.606873
O	2.108727	0.650446	0.620526
N	2.657657	1.432462	-0.350533
O	2.170315	2.587470	-0.498561
O	3.605550	0.974422	-0.997512
H	-2.130178	2.607002	-0.465553
N	-4.279368	0.037054	-0.630752
H	-3.832426	-2.004607	-0.216694
C	-2.868893	2.060778	-1.063699
H	-3.756202	2.688446	-1.220962
H	-5.560574	-1.532549	-0.044902
H	-2.411269	1.835613	-2.041278
H	-4.362067	-1.042076	1.195804
O	-2.378957	0.324919	0.560180
C	-4.523341	-1.219078	0.124300
C	-3.183762	0.761228	-0.348571
C	-5.249059	0.366166	-1.697783
H	-6.221191	0.634147	-1.254407
H	-5.382361	-0.515855	-2.342428
H	-4.892111	1.194369	-2.316971
O	-0.149826	2.350000	0.881350
H	0.689788	2.655151	0.416628
H	-0.081939	2.665259	1.804127
H	-0.628757	-3.061076	0.164232
H	-1.688078	-2.742600	1.267829

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Complex 1.2.2b

U	0.221765	0.782905	0.142207
O	0.500198	1.842246	-1.296210
O	-0.072518	-0.205456	1.634130
O	0.228807	-3.051303	-0.568146
O	-1.906821	-2.472732	-0.738454
O	-0.313422	-0.972003	-1.200605
N	-0.689842	-2.249328	-0.795497
O	2.383783	-0.205933	-0.058371
N	3.051860	-2.349571	0.248569
C	2.801258	-2.180547	1.702588
C	2.820002	-1.472210	-2.078238
C	3.359504	-3.717425	-0.218722
H	1.722139	-2.062127	1.881075
H	3.174842	-3.066471	2.228671
H	3.802907	-1.824231	-2.425490
H	3.320856	-1.286529	2.071943
H	2.605928	-0.492804	-2.521265
H	2.048948	-2.186835	-2.404123
H	4.203338	-4.116491	0.362292
H	2.475055	-4.357108	-0.074207
H	3.630203	-3.720640	-1.278744
C	2.754671	-1.332347	-0.570923
O	2.082746	2.178038	1.319654
H	-3.821980	1.163329	-2.708473
N	-3.892114	-0.307043	-0.271085
H	-3.850888	-1.791041	1.217739
C	-2.899357	0.717549	-2.305381
H	-2.731104	-0.250259	-2.801745
H	-4.685102	-0.274611	1.702383
H	-2.053923	1.381175	-2.520720
H	-2.888319	-0.333194	1.594086
O	-2.135640	1.122260	-0.036029
C	-3.824833	-0.693625	1.157714
C	-2.976436	0.513916	-0.804556
C	-4.858434	-1.068958	-1.091471
H	-5.156257	-0.504123	-1.981776
H	-5.755335	-1.260061	-0.486868
H	-4.408908	-2.028620	-1.392482
O	-0.584787	2.858168	1.501314
H	-0.536665	2.721894	2.468516
H	-1.535080	2.975476	1.293560
H	2.931493	1.743589	1.094695
H	2.140712	3.087992	0.965507

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Complex 1.2.2c

U	0.096332	-0.004301	0.255515
O	-0.512463	0.773823	-1.258690
O	0.576735	-0.753248	1.834355
O	-2.150565	-1.339707	0.078840
O	2.322227	0.363034	-0.423240
N	3.582433	2.203422	0.056691
C	3.726614	1.782730	1.470174
C	2.530794	2.013764	-2.189789
C	4.074288	3.565870	-0.251142
H	3.415135	0.740010	1.579623
H	4.776333	1.898143	1.774771
H	1.993143	2.972128	-2.120411
H	3.082109	2.418166	2.096409
H	1.889960	1.285498	-2.699111
H	3.449492	2.170783	-2.775633
H	3.324099	4.303006	0.073658
H	5.016078	3.730096	0.289466
H	4.263295	3.686331	-1.323107
C	2.826926	1.495295	-0.795245
O	0.557792	2.145597	1.061622
N	0.039156	3.280132	0.511813
O	-1.209279	3.443773	0.604520
O	0.821882	4.079574	-0.011779
H	2.806485	-3.714562	-2.144016
N	1.101573	-4.034729	0.163080
H	-0.041814	-3.375789	1.829551
C	2.733528	-2.925772	-1.378512
H	3.587520	-3.030233	-0.692216
H	-0.409886	-5.036747	1.242699
H	2.786645	-1.943798	-1.861590
H	-0.976682	-3.598667	0.328679
O	0.568249	-2.040344	-0.799381
C	-0.166037	-4.011263	0.939622
C	1.410694	-3.000356	-0.635019
C	1.997031	-5.183796	0.416160
H	2.905244	-5.124379	-0.190506
H	1.468600	-6.117455	0.169545
H	2.276799	-5.204356	1.481389
O	-2.001502	0.991053	1.445568
H	-1.911091	1.960074	1.181237
H	-1.901136	0.986138	2.418528
H	-2.412223	-1.447096	-0.857504
H	-2.790135	-0.699849	0.464099

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Complex 1.2.2d

U	0.252190	-0.287493	0.092690
O	1.008198	0.479879	1.544621
O	-0.440760	-1.059521	-1.387314
O	0.092327	-2.765178	0.989435
O	-0.744901	1.804461	-0.363026
N	-0.363991	4.044251	-0.292359
C	0.274935	4.010656	-1.632226
C	-1.476047	2.934096	1.652979
C	-0.466473	5.386862	0.318210
H	-0.429779	4.391965	-2.388463
H	1.160508	4.662580	-1.613142
H	-0.748645	3.248925	2.417306
H	0.571314	2.987575	-1.884708
H	-1.810982	1.916763	1.884868
H	-2.339117	3.616067	1.694062
H	0.543818	5.783927	0.504819
H	-0.987431	6.062384	-0.378323
H	-1.016230	5.359966	1.263204
C	-0.834053	2.918580	0.274364
O	2.225750	-1.475618	-0.236025
N	2.269683	-2.302196	-1.325173
O	1.900531	-3.483199	-1.153321
O	2.677540	-1.810207	-2.396669
H	-2.366452	-3.405119	1.752825
N	-3.645349	-1.344972	0.045579
H	-3.036244	0.607866	-0.526677
C	-2.884927	-2.505136	2.121479
H	-3.918822	-2.761620	2.387185
H	-4.576201	0.030529	-1.250419
H	-2.355647	-2.155480	3.016305
H	-2.994923	-0.602383	-1.835942
O	-1.828369	-0.554846	1.191245
C	-3.556377	-0.254193	-0.956118
C	-2.779828	-1.415755	1.070827
C	-4.692357	-2.357693	-0.220902
H	-4.501854	-3.284677	0.328353
H	-4.685035	-2.588716	-1.296208
H	-5.684411	-1.963076	0.051558
O	1.839654	0.885013	-1.631904
H	2.646904	1.215500	-1.187445
H	2.174430	0.114841	-2.163465
H	0.563247	-2.882554	1.839027
H	0.652634	-3.262178	0.334085

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Complex 2.2.0

U	0.012182	0.037798	-0.257444
O	-0.103424	-0.007248	1.541105
O	0.127188	0.082881	-2.056027
O	1.445285	-2.002400	-0.248796
O	0.664141	-4.090323	-0.319172
O	-0.722758	-2.343664	-0.331560
N	0.473399	-2.883133	-0.300924
O	-2.541103	-0.363873	-0.321298
O	-1.420888	2.078497	-0.266248
N	-0.448952	2.958993	-0.213974
O	-0.639370	4.166243	-0.196050
O	0.747163	2.419270	-0.182774
O	2.565422	0.440131	-0.193596
H	-2.788286	-1.204866	0.111904
H	-3.032698	0.349116	0.132620
H	2.812086	1.282382	-0.624670
H	3.057513	-0.271431	-0.649189

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Complex 2.1.1

U	0.178276	0.154963	-0.466734
O	0.300827	0.207464	1.341635
O	0.065096	0.096433	-2.265566
O	1.659578	-1.904592	-0.380996
O	0.919692	-3.982917	-0.052669
O	-0.496651	-2.269670	-0.238331
N	0.707242	-2.785273	-0.215417
O	-2.350389	-0.460507	-0.180542
O	-1.532604	1.992084	-0.309053
N	-0.698502	3.004869	-0.311158
O	-1.061330	4.167992	-0.175699
O	0.551392	2.653453	-0.470109
H	2.612195	1.316627	2.370021
N	4.440113	0.015109	0.426343
H	4.159585	-1.915780	-0.424144
C	3.088777	1.823699	1.515639
H	2.374762	2.558990	1.126195
H	5.731611	-1.109956	-0.801944
H	4.000645	2.333402	1.855351
H	4.206340	-0.573965	-1.592421
O	2.511826	0.697273	-0.548255
C	4.650283	-0.962356	-0.669481
C	3.344477	0.807628	0.412879
C	5.405561	-0.054011	1.536427
H	5.506170	-1.102718	1.859336
H	5.070700	0.536719	2.394643
H	6.394733	0.308956	1.210167
H	-2.435202	-1.280637	0.344631
H	-2.811852	0.251404	0.305286

41
Complex 2.0.2a

U	0.315870	-0.505788	0.527368
O	-0.405245	0.650557	-0.680534
O	1.031301	-1.652984	1.725940

O	0.413196	1.394565	2.213800
O	-1.236438	1.963347	3.605517
O	-1.443548	0.231944	2.212466
N	-0.780213	1.234867	2.725940
O	-1.764817	-1.768971	0.451133
N	-3.548886	-2.737988	-0.526882
C	-2.778347	-4.005763	-0.576617
C	-3.569366	-0.256560	-0.050276
C	-4.961544	-2.827420	-0.929177
H	-1.742071	-3.797903	-0.869023
H	-2.781589	-4.500909	0.408288
H	-2.856758	0.407800	-0.562621
H	-3.250228	-4.667048	-1.316581
H	-3.638560	0.103169	0.986568
H	-4.545147	-0.192627	-0.543845
H	-5.044005	-3.026624	-2.011067
H	-5.444508	-3.655301	-0.384060
H	-5.503043	-1.905962	-0.694708
C	-2.931521	-1.634312	-0.029901
O	0.179233	-2.343540	-1.224376
N	1.347743	-2.144022	-1.778261
O	1.756763	-2.796914	-2.736843
O	2.037534	-1.183407	-1.220579
H	1.460514	1.834592	-1.777293
N	3.535555	2.758875	0.505457
H	2.648448	2.343235	2.388437
C	2.553031	1.887608	-1.653527
H	2.962292	0.978325	-2.117127
H	3.887658	3.645017	2.382962
H	2.933288	2.780731	-2.161040
H	4.385761	1.923441	2.280383
O	2.339248	0.849146	0.507622
C	3.618273	2.657179	1.984112
C	2.818829	1.815908	-0.160328
C	4.337161	3.827354	-0.111967
H	3.924716	4.817858	0.144444
H	4.367629	3.725718	-1.201007
H	5.371789	3.771807	0.265202

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Complex 2.0.2b

U	0.619867	-0.076347	1.621735
O	-0.416620	0.785195	3.723225
O	1.374878	0.188648	-0.608913
O	-1.034208	0.021584	0.872813
O	2.283103	-0.169588	2.329169
O	-1.446390	-0.500505	5.229034
O	-0.426218	-1.401877	3.460522
O	0.714874	-2.368248	0.972870
O	0.093656	-0.729573	-2.192474
O	0.103895	1.469401	-1.926784
O	0.737207	2.302930	1.535085
N	-0.797386	-0.379181	4.195294
N	0.471893	0.315110	-1.620622
N	0.558588	-3.465349	-0.998332
N	0.595181	3.838553	-0.118786
C	-1.487545	3.149694	1.092582
C	0.007983	3.087513	0.834886
C	2.000093	-3.194802	-1.216416
C	-0.021647	-2.957008	0.107702
C	-1.517789	-3.064723	0.346263
C	2.034373	3.613370	-0.395711
C	-0.148602	4.583391	-1.148492
C	-0.192003	-3.936980	-2.174127
H	-1.680878	2.655788	2.052139
H	2.550426	-3.355142	-0.281860
H	-1.875627	4.178091	1.115582
H	2.369821	-3.878326	-1.992355
H	-2.031810	-2.321007	-0.282707
H	2.584541	3.541383	0.549856
H	2.123959	-2.148908	-1.533422
H	-2.007145	2.582113	0.304666
H	2.412198	4.458090	-0.987048
H	-1.706574	-2.811742	1.396236
H	-1.915708	-4.065340	0.124547
H	-1.198558	4.708460	-0.865686
H	-0.103001	4.027966	-2.098783
H	2.148576	2.671652	-0.952380
H	-0.140489	-3.172158	-2.965333
H	0.249809	-4.876405	-2.541413
H	-1.243259	-4.115547	-1.927129
H	0.302971	5.578777	-1.282275

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Complex 2.0.2c

U	7.145710	8.237192	6.549904
O	6.011504	8.950396	5.329526
O	8.289411	7.553064	7.792220
O	6.997150	6.160083	5.661206
N	7.689636	5.070796	6.186679
O	7.100705	4.401287	7.049841
O	8.816268	4.848555	5.716097
H	10.994788	7.533888	7.224879
N	10.823489	10.066265	5.795703
H	9.472733	11.068760	4.505338
C	10.967801	7.585627	6.125009
H	11.995253	7.536436	5.735843
H	10.701851	12.110186	5.302872
H	10.387475	6.727480	5.763984
H	9.303264	11.469605	6.243703
O	9.047385	8.778440	5.248740
C	10.019477	11.260419	5.436378
C	10.246183	8.852873	5.705073
C	12.086236	10.325433	6.508591
H	12.601664	9.390938	6.750926
H	11.863579	10.859426	7.445741
H	12.746729	10.944555	5.881300
O	7.809723	10.111288	9.878696
N	8.321135	10.306695	8.758421
O	7.485586	10.268945	7.669816
O	9.523481	10.560954	8.547643
H	7.235788	6.554959	10.146763
N	5.149673	8.586631	10.201857
H	4.077122	10.382554	10.446127
C	6.203243	6.343330	9.827124
H	6.251084	5.648686	8.979364
H	3.904121	9.615950	8.829433
H	5.654306	5.882625	10.661383
H	5.427585	10.458739	9.253632
O	5.393674	7.824927	8.087002
C	4.601405	9.847255	9.643544
C	5.558578	7.630249	9.346253
C	5.483231	8.603990	11.636567
H	6.233739	9.389171	11.818831
H	5.895688	7.642465	11.957568
H	4.577657	8.817825	12.225821

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Complex 2.0.2d

U	0.022495	-0.298416	0.163432
O	0.133124	-0.452250	-1.638296
O	-0.088165	-0.145486	1.965235
O	3.517440	-2.661536	0.541459
O	1.298890	-2.480544	0.394834
O	2.533084	-0.671192	0.349712
N	2.497119	-1.984258	0.434453
O	-1.325603	1.766680	0.008478
N	-3.558365	2.037813	-0.340777
C	-3.360784	1.764974	-1.781784
C	-2.687969	1.983305	1.997178
C	-4.942759	1.906576	0.148595
H	-2.346963	2.061305	-2.069289
H	-3.479558	0.685706	-1.971358
H	-3.221981	2.890066	2.320629
H	-4.102389	2.334724	-2.359893
H	-1.698906	1.938890	2.466399
H	-3.263244	1.101664	2.321195
H	-5.624763	2.386958	-0.567434
H	-5.209338	0.838975	0.240821
H	-5.068121	2.395595	1.121698

C	-2.489381	1.931142	0.490002
O	-1.285069	-2.470191	0.299545
N	-2.476052	-1.970814	0.174427
O	-3.505880	-2.642115	0.178876
O	-2.493359	-0.661599	0.039049
H	3.324640	0.671958	-2.196586
N	3.637218	2.037887	0.269923
H	4.188597	2.663385	2.210504
C	2.761945	1.603348	-2.025968
H	3.307730	2.435325	-2.497063
H	3.544009	0.980669	2.104778
H	1.771601	1.494121	-2.481666
H	2.429321	2.367658	1.969287
O	1.400075	1.744105	-0.030047
C	3.438753	2.014081	1.736212
C	2.565212	1.808376	-0.531625
C	5.018622	1.806606	-0.189958
H	5.149304	2.124828	-1.230856
H	5.269533	0.734785	-0.102850
H	5.708848	2.389503	0.436455

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Complex 2.0.2e

U	-0.218750	0.391875	-0.334752
O	-0.174125	0.982055	-2.045435
O	-0.245469	-0.251101	1.370473
O	-3.730053	2.523678	0.389138
O	-1.502042	2.406601	0.351367
O	-2.690356	0.663061	-0.274027
N	-2.695009	1.904788	0.168026
O	1.731339	-1.058595	-0.728881
N	3.620342	-1.247043	0.499990
C	2.839909	-2.016906	1.496818
C	3.637150	0.214237	-1.527295
C	5.008753	-0.906783	0.857352
H	2.560498	-3.001069	1.089277
H	3.459178	-2.158535	2.391246
H	3.883755	1.138696	-0.984177
H	1.923012	-1.470943	1.761445
H	2.921324	0.448963	-2.323594
H	4.553015	-0.211239	-1.965997
H	5.009826	-0.230236	1.725344
H	5.561137	-1.828365	1.100097
H	5.513523	-0.405108	0.026255
C	2.957410	-0.739006	-0.561348
O	1.505094	1.794653	0.221983
N	2.111457	1.949851	1.454176
O	1.452380	2.459674	2.364528
O	3.305348	1.578226	1.517648
H	-0.353695	-4.741502	-1.277205
N	-1.998845	-3.221936	0.534932
H	-2.558780	-1.505474	1.658889
C	0.043936	-3.846955	-0.771256
H	0.612095	-4.173821	0.112994
H	-3.850694	-2.740865	1.422378
H	0.721083	-3.309915	-1.443647
H	-3.357711	-1.650994	0.079556
O	-1.129701	-1.753451	-0.977555
C	-3.009354	-2.216563	0.950464
C	-1.072758	-2.881720	-0.390529
C	-1.974490	-4.476138	1.305628
H	-1.255850	-5.188523	0.888124
H	-2.973365	-4.939873	1.284286
H	-1.706032	-4.272177	2.356337

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Complex 2.0.2f

U	9.206445	7.683580	7.224813
O	8.527620	7.923881	8.894607
O	9.873399	7.449174	5.554422
O	10.126622	4.841023	9.804327
O	8.069324	4.457528	9.066775
O	9.555548	5.480646	7.735592
N	9.234915	4.901041	8.956915
O	8.473190	9.892455	6.679388
N	9.571235	11.845432	7.039304
C	10.538523	11.474724	5.979001
C	7.754043	11.161372	8.612588
C	9.963396	12.986953	7.884815
H	10.022870	10.926593	5.182912
H	10.990843	12.390963	5.576602
H	8.381364	11.052275	9.510995
H	11.311847	10.822487	6.414918
H	6.993149	10.373163	8.622844
H	7.270185	12.149302	8.626924
H	9.173735	13.240279	8.599076
H	10.875263	12.727112	8.444874
H	10.154507	13.862160	7.245380
C	8.626192	10.949326	7.387894
O	11.890141	8.536100	9.989892
N	11.315777	9.260484	9.176104
O	10.922554	10.433519	9.367737
O	11.115364	8.749676	7.899672
O	7.051961	6.915264	6.530594
N	6.211994	4.813183	6.688028
C	7.149586	4.379889	5.624773
C	5.539294	6.524031	8.380894
C	5.539291	3.726840	7.422220
H	8.125971	4.153476	6.081804
H	6.739312	3.487633	5.133297
H	5.982845	6.031571	9.260281
H	7.280373	5.186735	4.895374
H	4.467130	6.282087	8.333154
H	5.673148	7.606419	8.485059
H	5.004960	3.083285	6.706879
H	6.292665	3.135795	7.966087
H	4.817962	4.123847	8.143323
C	6.300006	6.078642	7.144606

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TS 2.0.2a-2.0.2b

U	0.016776	0.440566	-0.474402
O	-1.008286	2.676183	0.073463
O	0.680872	-1.877847	-0.976312
O	0.177642	0.202281	1.320013
O	-0.106684	0.726140	-2.252958
O	0.160660	4.529787	0.496820
O	1.174324	2.653031	-0.161156
O	2.430702	0.198052	-0.535947
O	0.249683	-3.874930	-0.105724
O	-1.133094	-2.163817	0.248622
O	-2.386055	0.323942	-0.387976
N	0.111727	3.351779	0.153985
N	-0.081332	-2.688656	-0.258705
N	3.762654	-1.325019	0.510994
N	-3.993148	-1.042063	0.441904
C	-2.984288	0.710543	1.924263
C	-3.116506	-0.022117	0.598120
C	3.641001	-2.279262	-0.616934
C	3.143957	-0.120639	0.472575
C	3.288603	0.862419	1.627475
C	-4.031956	-1.773486	-0.844852
C	-4.704610	-1.696264	1.552010
C	4.529307	-1.822270	1.665674
H	-2.518743	1.682219	1.720308
H	3.300669	-1.744071	-1.507683
H	-3.944076	0.859355	2.437492
H	4.627654	-2.735131	-0.794386
H	2.653055	0.536006	2.466030
H	-3.759572	-1.093287	-1.658509
H	2.899061	-3.056477	-0.379673
H	-2.303421	0.142165	2.577794
H	-5.050235	-2.159065	-0.999313
H	2.914859	1.833068	1.282159
H	4.326857	0.961672	1.975354
H	-4.609777	-1.124988	2.480241
H	-4.279907	-2.701308	1.715591
H	-3.310132	-2.604443	-0.816089
H	4.176621	-2.835363	1.916826
H	5.604369	-1.877572	1.422322

H	4.392173	-1.184662	2.544439
H	-5.773321	-1.798615	1.304052

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TS 2.0.2b-2.0.2c

U	-0.036515	0.612327	-0.532783
O	-1.820396	2.981516	1.092746
O	0.330830	-1.715671	-0.564875
O	-0.081517	0.427837	1.274990
O	0.045921	0.714349	-2.339701
O	-0.217248	4.518364	1.129175
O	-0.144846	2.889493	-0.396601
O	2.337661	0.655704	-0.361234
O	1.484980	-2.598186	1.133981
O	-0.713590	-2.859940	1.047206
O	-2.318069	-0.015327	-0.594592
N	-0.758432	3.502443	0.685963
N	0.367523	-2.419759	0.606702
N	3.824378	-1.009675	0.015514
N	-3.364410	-1.952204	-0.084292
C	-3.198293	-0.165377	1.661313
C	-2.948951	-0.720871	0.272291
C	3.627465	-1.458147	-1.383731
C	3.068890	0.010513	0.469838
C	3.059545	0.392266	1.939113
C	-2.937871	-2.479698	-1.402869
C	-3.901686	-2.942930	0.863804
C	4.550875	-1.944522	0.891620
H	-2.939585	0.899054	1.651994
H	3.548883	-0.587202	-2.044458
H	-4.239057	-0.300580	1.990169
H	4.484102	-2.078524	-1.678471
H	2.537184	-0.395976	2.503681
H	-3.079466	-1.711546	-2.172340
H	2.693059	-2.037521	-1.444186
H	-2.527238	-0.675690	2.370467
H	-3.544014	-3.364159	-1.638666
H	2.493468	1.324233	2.044092
H	4.071379	0.521294	2.350779
H	-4.200396	-2.468609	1.803658
H	-3.125936	-3.694915	1.078332
H	-1.871413	-2.746259	-1.353900
H	3.978836	-2.881921	0.975721
H	5.542284	-2.152561	0.460592
H	4.684948	-1.524946	1.893430
H	-4.780715	-3.436373	0.420863

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Complex 2.0.1

U	-0.028899	-0.753873	0.601550
O	-0.938373	0.144315	-0.681977
O	0.841787	-1.674557	1.883886
O	0.684787	1.384010	1.569170
O	-0.490346	2.571541	3.048610
O	-1.239241	0.604002	2.307601
N	-0.357669	1.576838	2.350175
O	-2.023539	-1.963182	0.940240
N	-3.551247	-2.744564	-0.540678
C	-2.712829	-3.951926	-0.753531
C	-3.927542	-0.521832	0.555274
C	-4.733673	-2.617463	-1.411744
H	-1.929939	-3.746897	-1.498933
H	-2.226662	-4.231035	0.188094
H	-3.755236	0.167430	-0.287520
H	-3.361424	-4.768338	-1.098791
H	-3.534746	-0.044226	1.460656
H	-5.006391	-0.700110	0.664073
H	-4.422929	-2.743519	-2.461211
H	-5.471906	-3.398184	-1.165770
H	-5.201841	-1.634051	-1.307333
C	-3.132759	-1.793601	0.317016
O	0.237775	-2.644227	-1.010040
N	1.369588	-2.219760	-1.527852
O	1.947523	-2.802686	-2.434826
O	1.821539	-1.111900	-0.984468

44
Complex 2.1.2a

U	0.000000	-0.000000	0.000000
O	-1.281845	1.217369	-0.421337
O	1.328800	-1.168866	0.387758
O	-1.279907	-2.943297	2.330309
O	-0.802006	-1.332989	3.775724
O	-1.392731	-0.803135	1.695196
N	-1.131634	-1.747834	2.640497
O	-1.273769	-1.762822	-1.010727
N	-2.899904	-3.132874	-1.760639
C	-2.567329	-4.091456	-0.679741
C	-2.579874	-0.871048	-2.827112
C	-3.889034	-3.602211	-2.743999
H	-2.149351	-3.558775	0.182619
H	-3.489378	-4.615504	-0.386181
H	-1.769646	-0.788796	-3.568720
H	-1.833099	-4.832829	-1.037706
H	-2.583527	0.080272	-2.274635
H	-3.544601	-0.999161	-3.330889
H	-3.620249	-4.622042	-3.064472
H	-4.897980	-3.632451	-2.298052
H	-3.906698	-2.962222	-3.631638
C	-2.228075	-1.954937	-1.827747
O	0.543648	-0.066700	-2.375994
N	0.496716	0.896652	-3.293545
O	1.065617	2.012100	-3.033749
O	-0.069622	0.667049	-4.374207
H	-1.629249	2.936714	3.614046
N	0.547077	1.330791	4.270128
H	1.634289	-0.487580	4.294817
C	-1.471260	2.043781	2.990992
H	-2.149437	1.243743	3.325171
H	2.371422	0.868923	5.226015
H	-1.697529	2.275497	1.943850
H	2.429085	0.862789	3.430010
O	0.598210	1.256229	2.002367
C	1.831333	0.597099	4.308123
C	-0.046898	1.522357	3.065470
C	-0.214813	1.353088	5.531885
H	-0.987968	2.129798	5.512480
H	0.472721	1.575199	6.360624
H	-0.690418	0.372955	5.703131
O	1.834847	1.669689	-0.530531
H	1.642788	1.914348	-1.497801
H	2.677853	1.176914	-0.550672

44
Complex 2.1.2b

U	0.000000	0.000000	0.000000
O	-1.342846	1.001305	-0.672863
O	1.464455	-0.858952	0.633944
O	-0.280167	-2.232861	2.906088
O	-2.151716	-1.337318	3.687586
O	-1.454182	-0.762131	1.665991
N	-1.278133	-1.491508	2.805246
O	1.145264	0.113941	-2.143906
N	0.798546	-1.227577	-3.951191
C	1.607994	-2.312927	-3.345776
C	-0.303333	1.009987	-3.867365
C	0.031155	-1.610546	-5.154930
H	0.946480	-3.146278	-3.067295
H	2.353069	-2.653042	-4.082037
H	0.033367	1.327438	-4.866617
H	2.104774	-1.933865	-2.448494
H	-0.288418	1.862366	-3.179314
H	-1.335045	0.635696	-3.934443
H	0.677647	-2.212608	-5.810110
H	-0.843529	-2.210297	-4.855379
H	-0.302864	-0.727741	-5.710064
C	0.592411	-0.070541	-3.283291
O	-0.668415	-1.950069	-1.107285
N	-1.475643	-2.180618	-2.178368
O	-2.193148	-1.253922	-2.612301
O	-1.407944	-3.324989	-2.677139
H	-1.670452	2.467033	4.385576

N	0.483536	0.716030	4.068331
H	1.671749	-0.811172	3.189760
C	-1.609489	1.923264	3.431078
H	-2.304060	1.067741	3.457483
H	2.382343	0.003685	4.633600
H	-1.896858	2.585819	2.606531
H	2.333466	0.839596	3.044149
O	0.287441	1.591244	1.973188
C	1.805122	0.148407	3.710234
C	-0.214420	1.402119	3.135374
C	-0.078102	0.247250	5.351671
H	-1.061325	0.686890	5.537481
H	0.604500	0.518719	6.172411
H	-0.196461	-0.846725	5.309389
O	1.640614	2.065880	-0.230225
H	2.497063	1.658688	-0.464392
H	1.682678	2.281067	0.727373

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Complex 2.1.2c

U	-0.235803	0.245220	-0.708742
O	-0.475903	0.832222	-2.400126
O	0.032083	-0.324389	0.997768
O	-3.810019	0.113043	1.572373
O	-2.496615	1.877188	1.826232
O	-2.451080	0.706738	-0.082855
N	-2.938021	0.894832	1.163745
O	1.404168	-1.531331	-1.365332
N	3.165484	-2.106981	-0.032311
C	2.248126	-2.566438	1.031675
C	3.593766	-0.968124	-2.210978
C	4.583695	-2.034619	0.364612
H	1.291561	-2.866806	0.593005
H	2.710914	-3.415590	1.556023
H	4.025525	-0.042992	-1.800384
H	2.051001	-1.748258	1.741304
H	2.989577	-0.718105	-3.090433
H	4.404153	-1.654252	-2.500363
H	4.687642	-1.348157	1.218776
H	4.938158	-3.038422	0.650410
H	5.204785	-1.655196	-0.450788
C	2.662164	-1.558505	-1.166198
O	1.951082	1.210405	-0.627149
N	2.676077	1.465621	0.474920
O	2.199451	2.254169	1.336313
O	3.799872	0.930069	0.568909
H	-0.994747	-4.890411	-2.123587
N	-1.551895	-3.525124	0.254428
H	-1.558517	-2.079023	1.819862
C	-0.460261	-3.942780	-1.958191
H	0.564253	-4.163469	-1.620571
H	-2.917617	-3.261764	1.838842
H	-0.391255	-3.385820	-2.898804
H	-2.888234	-1.917789	0.652439
O	-1.390568	-1.831522	-1.262695
C	-2.274836	-2.639636	1.201035
C	-1.163986	-3.041218	-0.950724
C	-1.237034	-4.875403	0.747786
H	-0.588949	-5.416629	0.051042
H	-2.163088	-5.455112	0.898671
H	-0.715594	-4.795590	1.715965
O	-0.349026	2.544426	0.261228
H	0.499228	2.651518	0.767905
H	-1.099557	2.512565	0.917517

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Complex 2.1.2d

U	-0.002769	-0.001404	-0.005044
O	0.018878	-0.009317	2.500587
O	1.801813	0.006323	0.090773
O	-1.817484	-0.016883	-0.075681
O	-0.305563	1.948752	1.573512
O	0.246251	2.227261	-0.985510
O	-0.483208	-2.202245	0.969376
O	0.734323	-2.052433	-1.514537
N	-0.232372	1.265428	2.683773
C	-1.516694	-2.915584	0.763774
C	-0.085756	2.769072	-2.086822
H	-0.025278	-2.080767	-2.174482
H	1.495342	-1.699543	-2.014764
O	-0.391426	1.760590	3.796435
N	-1.361356	3.144590	-2.336990
N	-2.638291	-2.742091	1.504487
C	-1.476385	-3.966314	-0.338840
C	0.994141	2.989613	-3.135897
C	-2.420666	2.817537	-1.357967
C	-2.683870	-1.700508	2.555248
C	-3.925049	-3.400443	1.223808
C	-1.841924	3.453953	-3.698392
H	-1.904867	-4.931766	-0.033409
H	-2.024134	-3.589521	-1.218857
H	1.964451	2.818775	-2.654899
H	-0.427122	-4.095630	-0.625470
H	0.975106	3.997059	-3.577519
H	0.860088	2.247050	-3.938799
H	-3.219209	3.568525	-1.444640
H	-2.822264	1.814790	-1.568763
H	-3.082454	-0.764834	2.133095
H	-2.004763	2.830658	-0.345066
H	-1.675135	-1.506304	2.932764
H	-4.688114	-2.631455	1.018147
H	-4.249220	-3.990721	2.097264
H	-3.335982	-2.052008	3.368341
H	-1.050488	3.903110	-4.308309
H	-2.192203	2.522539	-4.172285
H	-2.674480	4.169675	-3.631817
H	-3.859493	-4.058606	0.352524
O	-0.492384	0.191084	-2.570427
N	-1.517651	-0.481498	-3.057829
O	-2.442077	0.129668	-3.629805
O	-1.516272	-1.759803	-2.936573

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Complex 1.1.2a…NO_3^-

U	0.000017	0.000891	0.001692
O	0.005187	-0.005252	2.485370
O	1.805400	0.002435	-0.069316
O	-1.807821	-0.007490	0.064553
O	-0.057214	1.974704	1.521841
O	-0.195348	1.859945	-1.462553
O	-0.211068	-2.314607	0.544413
O	-0.214166	-1.152267	-2.189873
N	-0.085765	1.296027	2.645898
C	-1.181712	-3.079453	0.189963
C	-0.965434	2.359236	-2.360794
H	-1.210716	-1.471206	-2.257234
H	-0.159913	-0.562097	-2.968346
O	-0.191971	1.826431	3.744713
N	-2.190135	2.833103	-2.072658
N	-2.357752	-3.086419	0.846539
C	-0.967596	-4.021697	-0.984960
C	-0.417265	2.447404	-3.778872
C	-2.742045	2.768643	-0.698732
C	-2.594864	-2.205934	2.012764
C	-3.563741	-3.705501	0.244767
C	-3.204382	3.112195	-3.113832
H	-1.048700	-5.072364	-0.661969
H	-1.709883	-3.842610	-1.775631
H	0.643359	2.169747	-3.744737
H	0.033643	-3.834889	-1.387490
H	-0.507116	3.464549	-4.189979
H	-0.958957	1.752817	-4.436661
H	-3.376004	3.654539	-0.546554
H	-3.341337	1.853671	-0.590430
H	-3.168938	-1.321736	1.700562
H	-1.932166	2.765923	0.037251
H	-1.640558	-1.873270	2.432498
H	-3.915418	-3.067712	-0.582868
H	-4.338215	-3.782837	1.018523
H	-3.157187	-2.775182	2.768022

H	-2.740535	3.279796	-4.090106
H	-3.872335	2.238817	-3.178460
H	-3.770007	4.012113	-2.829333
H	-3.346806	-4.715709	-0.126902
O	-2.422285	0.115395	-3.469216
N	-3.157576	-0.531016	-2.647288
O	-4.262706	-0.097724	-2.242412
O	-2.715590	-1.696158	-2.214456

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Complex 2.0.2b…H_2O

U	-0.000681	0.002159	0.004973
O	0.013946	-0.004132	2.488914
O	1.812690	0.000873	-0.113743
O	-1.818110	-0.020247	0.077611
O	-0.046691	1.972159	1.516730
O	-0.074048	1.916589	-1.432314
O	0.081954	-2.278764	0.626598
O	-0.312248	-1.011495	-2.113561
N	-0.060852	1.298922	2.644535
C	-0.521960	-3.347709	0.266525
C	-0.683276	2.084304	-2.543779
N	-1.561217	-1.362858	-2.558371
O	-0.139908	1.836222	3.742453
N	-1.965767	2.506993	-2.562692
N	-1.723394	-3.662057	0.799361
C	0.150033	-4.267995	-0.734216
C	0.069802	1.799827	-3.831523
O	-2.111114	-0.590493	-3.368955
O	-2.045611	-2.431785	-2.140158
C	-2.687596	2.723827	-1.287856
C	-2.400841	-2.708098	1.708105
C	-2.549926	-4.759889	0.261233
C	-2.810340	2.493886	-3.770640
H	0.369506	-5.250078	-0.283982
H	-0.503221	-4.414829	-1.606252
H	1.129934	1.686741	-3.576977
H	1.081179	-3.789422	-1.069056
H	-0.046839	2.596328	-4.581059
H	-0.301009	0.850173	-4.245087
H	-3.425528	3.525175	-1.436022
H	-3.191941	1.795488	-0.979705
H	-3.002062	-1.993399	1.125824
H	-1.976153	3.007066	-0.504450
H	-1.653530	-2.144696	2.278154
H	-3.133470	-4.405579	-0.604781
H	-3.237173	-5.106258	1.045589
H	-3.044443	-3.274378	2.395532
H	-2.207646	2.376103	-4.675595
H	-3.513412	1.647732	-3.712389
H	-3.374111	3.437538	-3.835698
H	-1.926123	-5.606426	-0.048191
O	2.368830	-2.284166	-2.137952
H	1.499890	-1.945390	-2.436996
H	2.577955	-1.675088	-1.401369

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TS 1.1.2a…NO_3^--2.1.2d

U	0.152289	0.542939	-0.600927
O	1.771318	2.318470	0.074987
O	-1.821518	-1.684317	-0.407508
O	0.043749	1.365751	-2.204381
O	0.321350	-0.282420	1.004617
O	1.280722	4.086827	1.345366
O	-0.302257	2.648158	0.705037
O	-2.192842	1.039880	-0.332736
O	-1.834310	-3.161095	1.249771
O	-0.243986	-3.250892	-0.296266
O	2.453283	-0.225287	-0.782225
N	0.932946	3.076857	0.741550
N	-1.311546	-2.709327	0.207297
N	-3.502883	0.083670	1.295849
N	3.496105	-1.087480	1.060774
C	2.992844	-2.575432	-0.878920
C	2.973085	-1.223023	-0.180047
C	-2.461035	0.300747	2.323073
C	-3.259494	0.431435	0.013130
C	-4.279083	0.114724	-1.070268
C	3.445140	0.218396	1.756167
C	3.964285	-2.214711	1.885613
C	-4.482187	-0.970977	1.635453
H	3.982510	-3.054704	-0.849112
H	-2.955501	0.406968	3.299359
H	2.252979	-3.241976	-0.405589
H	-1.775911	-0.560607	2.338825
H	-4.011509	0.694767	-1.961599
H	2.523604	0.283392	2.355036
H	-1.894138	1.209336	2.094643
H	2.685724	-2.412184	-1.917263
H	3.438895	1.032599	1.025272
H	-5.311693	0.351915	-0.774590
H	-4.212556	-0.958373	-1.308783
H	3.354562	-2.270608	2.802529
H	5.017775	-2.060789	2.172467
H	4.324666	0.299812	2.411255
H	-5.342489	-0.951596	0.957631
H	-3.975003	-1.948623	1.569987
H	-4.844864	-0.806486	2.660312
H	3.874329	-3.167063	1.355504
O	0.335708	-1.492738	-2.140790
H	0.100727	-2.280108	-1.525150
H	-0.396114	-1.447778	-2.785891

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TS 2.1.2d-2.0.2b

U	0.038977	0.413995	-0.637222
O	1.479205	2.445293	-0.282409
O	-0.063556	0.838157	-2.390682
O	0.095554	-0.016435	1.129135
O	-0.666888	2.725531	0.064601
O	-2.375486	0.713698	-0.468622
O	2.376757	-0.148914	-0.470436
O	1.239261	-1.925804	-2.456005
N	0.526187	3.260641	0.101329
C	3.039285	-0.928397	0.286750
C	-3.222460	-0.036298	0.117113
H	0.860264	-2.581198	-1.828010
H	0.507375	-1.743858	-3.075191
O	0.738738	4.412805	0.467660
N	-3.444897	0.062467	1.449917
N	3.404764	-0.540069	1.532204
C	3.420195	-2.304659	-0.238792
C	-4.013102	-1.044964	-0.701378
C	-2.657852	1.011249	2.268796
C	3.067322	0.813974	2.028137
C	4.033482	-1.432048	2.521517
C	-4.210784	-0.959336	2.191954
H	4.451695	-2.590524	0.012024
H	2.725184	-3.054778	0.173362
H	-3.750069	-0.899289	-1.754396
H	3.284662	-2.285953	-1.325801
H	-5.099986	-0.923116	-0.570126
H	-3.724018	-2.061534	-0.397787
H	-3.301353	1.396418	3.073507
H	-1.779547	0.504950	2.697002
H	2.107040	0.787816	2.565281
H	-2.308770	1.837893	1.641087
H	2.974369	1.508840	1.187135
H	3.448014	-1.399955	3.454633
H	5.062409	-1.100446	2.742299
H	3.868253	1.145002	2.705556
H	-5.076252	-1.304607	1.613643
H	-3.564635	-1.822421	2.419864
H	-4.578597	-0.516898	3.128090
H	4.056777	-2.468051	2.170271
O	-1.053872	-1.725729	-0.833734
N	-0.849566	-2.704939	0.066146
O	-1.723780	-2.911901	0.930419
O	0.211484	-3.379159	-0.052398

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Complex 2.3.0

U	-0.519928	-0.147076	0.363530
O	0.127683	-0.910841	1.866713
O	-1.060589	0.569637	-1.206530
O	1.749119	2.278092	-1.305456
O	0.240882	3.607689	-0.354536
O	0.833542	1.708542	0.650548
N	0.937580	2.584756	-0.392337
O	-0.841908	-2.324709	-0.984924
O	-2.648121	-0.951646	0.727613
N	-3.587059	-0.752126	-0.247340
O	-4.290944	0.269158	-0.163230
O	-3.660285	-1.628022	-1.140125
O	1.642192	-0.526673	-0.971867
O	-1.969104	1.765690	1.265755
H	-2.877165	1.621133	0.912118
H	-1.627015	2.598369	0.872779
H	-1.828331	-2.373602	-1.094880
H	-0.484901	-2.185308	-1.884472
H	2.397462	-0.820891	-0.425247
H	1.861547	0.414684	-1.231147

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Complex 2.2.1

U	-0.439245	0.155773	-0.175322
O	-0.287042	-0.725727	-1.753839
O	-0.493152	1.008007	1.419556
O	-2.319276	-2.505882	2.600239
O	-3.410904	-0.713162	1.890754
O	-1.753795	-1.589581	0.656260
N	-2.521751	-1.601282	1.779567
O	1.856013	1.418117	-0.341397
O	-0.640671	2.194011	-1.297707
N	-0.683365	3.339385	-0.571994
O	-1.800561	3.783623	-0.251278
O	0.421453	3.874171	-0.291665
H	2.003034	-2.177506	-2.146291
N	1.561887	-3.464949	0.454122
H	1.049267	-2.872168	2.426115
C	2.634468	-1.984785	-1.264537
H	3.538019	-2.608455	-1.319764
H	0.912400	-4.630696	2.085971
H	2.911759	-0.923598	-1.281251
H	-0.322175	-3.468381	1.469291
O	1.355530	-1.217920	0.643384
C	0.744016	-3.622054	1.686386
C	1.819359	-2.224335	-0.003190
C	1.919819	-4.704742	-0.256944
H	2.392232	-4.489106	-1.220345
H	1.005489	-5.290557	-0.443026
H	2.607813	-5.309877	0.356020
O	-2.874267	0.837358	-0.330070
H	-2.927477	1.815893	-0.253901
H	-3.284653	0.432010	0.482765
H	1.580096	2.371902	-0.425306
H	2.245624	1.336252	0.550853

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Complex 2.0.1

U	-0.028899	-0.753873	0.601550
O	-0.938373	0.144315	-0.681977
O	0.841787	-1.674557	1.883886
O	0.684787	1.384010	1.569170
O	-0.490346	2.571541	3.048610
O	-1.239241	0.604002	2.307601
N	-0.357669	1.576838	2.350175
O	-2.023539	-1.963182	0.940240
N	-3.551247	-2.744564	-0.540678
C	-2.712829	-3.951926	-0.753531
C	-3.927542	-0.521832	0.555274
C	-4.733673	-2.617463	-1.411744
H	-1.929939	-3.746897	-1.498933
H	-2.226662	-4.231035	0.188094
H	-3.755236	0.167430	-0.287520
H	-3.361424	-4.768338	-1.098791
H	-3.534746	-0.044226	1.460656
H	-5.006391	-0.700110	0.664073
H	-4.422929	-2.743519	-2.461211
H	-5.471906	-3.398184	-1.165770
H	-5.201841	-1.634051	-1.307333
C	-3.132759	-1.793601	0.317016
O	0.237775	-2.644227	-1.010040
N	1.369588	-2.219760	-1.527852
O	1.947523	-2.802686	-2.434826
O	1.821539	-1.111900	-0.984468

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Complex 1.0.2

U	-0.169850	0.669221	-0.351877
O	-0.296075	0.543984	1.448102
O	-0.035412	0.644504	-2.144029
O	-2.104244	-0.610512	-0.430188
N	-4.170950	-0.235783	0.430908
C	-4.414756	0.807611	-0.602779
C	-2.711748	-1.997690	1.451474
C	-5.243502	-0.406372	1.437595
H	-4.007540	1.773596	-0.268631
H	-3.928612	0.519003	-1.541636
H	-1.937198	-2.647498	1.025103
H	-5.497986	0.892918	-0.756591
H	-3.585218	-2.606592	1.716562
H	-2.302700	-1.534098	2.364887
H	-5.548296	0.589023	1.793031
H	-6.113025	-0.903849	0.979965
H	-4.897292	-0.987621	2.297475
C	-3.013508	-0.908049	0.443060
O	-1.631784	2.602610	-0.344273
N	-0.683634	3.518487	-0.213269
O	-0.910009	4.708139	-0.130254
O	0.529958	2.998214	-0.180533
H	2.100821	1.295895	2.383025
N	4.285325	-0.039679	0.475028
H	3.618081	-0.939282	-1.326250
C	2.915239	1.641326	1.726152
H	2.557465	2.562720	1.240879
H	4.576280	-2.014873	-0.252786
H	3.803418	1.869416	2.322977
H	5.392733	-0.721667	-1.190037
O	2.128742	0.338152	-0.141928
C	4.474644	-0.992051	-0.647926
C	3.118572	0.600383	0.647091
C	5.463229	0.174654	1.357274
H	5.177784	0.123301	2.415863
H	5.940455	1.143625	1.144910
H	6.186777	-0.625212	1.159390