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Brønsted Acidity of Bio-Protic Ionic Liquids: The Acidic Scale of [AA]X Amino Acid Ionic Liquids

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Contents:

Table S1. The Hammett functions for AAILs and the contrastive compounds in water.

Compound	A_{max}(solvent)	A_{max}(Compound)	H_0
[Gly]NO_3	0.69705	0.67298	2.44
[Ala]NO_3	0.69705	0.67145	2.41
[Phe]NO_3	0.69705	/	/
[Asn]NO_3	0.69705	0.66757	2.34
[Ser]NO_3	0.69705	0.66529	2.31
[Thr]NO_3	0.69705	0.66560	2.32
[Val]NO_3	0.69705	0.67248	2.43
[Ile]NO_3	0.69705	0.67272	2.42
[Leu]NO_3	0.69705	0.67227	2.43
[Pro]NO_3	0.69705	0.66210	2.26
[His]$(NO_3)_2$	0.69705	0.64687	2.10
[Arg]$(NO_3)_2$	0.69705	0.65771	2.21
[Lys]$(NO_3)_2$	0.69705	0.66238	2.27
[Asp]$(NO_3)_2$	0.69705	0.65410	2.17
[Sar]NO_3	0.69705	0.66803	2.35
[DMGly]NO_3	0.69705	0.66808	2.35
[Bet]NO_3	0.69705	0.65395	2.17
EAN	0.69705	0.69079	3.04
[Et_3H]NO_3	0.69705	0.69221	3.14
Gly	0.69705	0.69064	3.02
Pro	0.69705	0.69328	3.25

Concentrations of compound: 0.010 mol L^{-1}; indicator: 5.0x10^{-5} mol L^{-1}. All tests are carried out at 25.0(±0.1) °C.

Table S2. The Hammett functions for [Pro]NO_3 in water.

Concentration	A_{max} (solvent)	A_{max}(Compound)	H_0
0	0.69705	0	\
0.0010	0.69705	0.69203	3.13
0.0025	0.69705	0.68829	2.89
0.0050	0.69705	0.68045	2.6
0.00750	0.69705	0.66985	2.42
0.0100	0.69705	0.66715	2.34
0.0250	0.69705	0.63567	2.01
0.0500	0.69705	0.59671	1.76
0.0750	0.69705	0.57542	1.66
0.1000	0.69705	0.54946	1.56

Indicator: 5.0×10^{-5} mol L^{-1}. All tests are carried out at 25.0(±0.1) °C.

Table S3. The Hammett functions for [Gly]NO_3 in water.

Concentration	**A_{max} (solvent)**	**A_{max}(Compound)**	H_0
0	0.69705	0	\
0.0010	0.69705	0.69293	3.23
0.0025	0.69705	0.68984	2.97
0.0050	0.69705	0.68418	2.72
0.00750	0.69705	0.67814	2.54
0.0100	0.69705	0.67298	2.44
0.0250	0.69705	0.65238	2.15
0.0500	0.69705	0.62431	1.92
0.0750	0.69705	0.61143	1.84
0.1000	0.69705	0.59898	1.78

Indicator: 5.0×10^{-5} mol L^{-1}. All tests are carried out at 25.0(±0.1) °C.

The optimized geometry coordinates (Å) (M06/6-311++G(d,p) level)

$Gly^{+}(H_2O)_3$

N	0.92063900	-0.00323200	-0.33559800
H	0.66654500	0.86393900	-0.84679800
C	0.17104100	-0.04507600	0.93869400
H	0.41471000	-0.95966000	1.47990100
C	-1.31438700	-0.00650300	0.64799900
O	-1.77767600	0.06057400	-0.45988400
O	-2.01162500	-0.05460900	1.76924700
H	0.64633600	-0.82222100	-0.90973000
H	1.93742300	-0.02137700	-0.14404100
O	-0.34278800	-2.25495300	-1.32209200
H	-0.15221700	-3.12285000	-1.68953700
H	-1.23038100	-2.01597700	-1.61058200
O	-0.25648000	2.34217400	-1.20175200
H	-0.04613300	3.21500800	-1.54551200
H	-1.15805100	2.13963100	-1.47479100
H	-2.95957800	-0.02571000	1.56883400
H	0.44564600	0.81105700	1.55558000
O	3.58343000	-0.04633300	0.58790700
H	4.15274400	0.71494600	0.73555000
H	4.13966700	-0.81951400	0.72274800

$Gly^{+-}(H_2O)_3$

N	0.88234100	-0.46465100	0.06284900
H	0.51736400	-1.03709400	-0.72026200
C	0.39524500	0.94151600	-0.07918500
H	0.81411900	1.53446700	0.73268200
C	-1.16046200	1.04634900	-0.04852400
O	-1.77817500	-0.06602400	-0.04934200
O	-1.58990400	2.18406300	-0.03354300
H	0.50528700	-0.87572600	0.93562500
H	1.90704900	-0.48076800	0.07016400
O	-0.83472500	-1.43458600	2.01647500
H	-1.19823000	-1.32205400	2.89600500
H	-1.45511800	-1.00914400	1.38194200
O	-0.66546200	-1.47196800	-1.99480900
H	-1.06043700	-2.17904100	-2.50577000
H	-1.36167900	-1.06292600	-1.43399600
H	0.75655000	1.33122200	-1.03094500
O	3.68819800	0.22695800	0.05622300
H	3.91105600	1.10734700	-0.25682800
H	4.51949900	-0.18847000	0.29766100

$Ala^{+}(H_2O)_3$

N	0.79789500	0.46043000	0.36379200
H	0.57143500	0.00629800	1.26970100
C	0.16458600	-0.31267500	-0.74011200
H	0.37155600	0.21270800	-1.67536200
C	0.71164600	-1.73605300	-0.78398800
C	-1.33725300	-0.28745900	-0.51402500
H	0.49967300	-2.25265900	0.15438600
H	0.24322700	-2.28054000	-1.60263600
H	1.78911900	-1.71002800	-0.95010500
O	-1.86650000	0.19738600	0.45305600
O	-1.97673100	-0.87383700	-1.51261800
H	0.41441500	1.42343700	0.37509600
H	1.82174800	0.48434300	0.22367100
O	-0.71073500	2.75656900	-0.04679400
H	-0.63043900	3.70212400	-0.20081000
H	-1.59702900	2.60079900	0.29710100
O	-0.28672500	-1.01510900	2.46321300
H	-0.08439600	-1.41198000	3.31513700
H	-1.22092200	-0.77791600	2.47339000
H	-2.93096000	-0.85650100	-1.34412400
O	3.55119700	0.30444300	-0.33403000
H	4.00169200	0.83514400	-0.99815900
H	4.24770100	-0.13674800	0.16230800

$Ala^{+-}(H_2O)_3$

N	0.75727100	0.60642900	0.04852400
H	0.47337600	0.65701200	1.04368700
C	0.26189000	-0.68373600	-0.54262500
H	0.57616600	-0.69196900	-1.58770500
C	0.87187300	-1.85311000	0.21399700
C	-1.29758200	-0.74859700	-0.50634000
H	0.58666200	-1.80893800	1.26855900
H	0.48175500	-2.77642600	-0.21241700
H	1.96200700	-1.85598500	0.13337600
O	-1.87000000	0.17140300	0.16397700
O	-1.78303900	-1.68466700	-1.11532600
H	0.31455000	1.41143300	-0.42813300
H	1.77904600	0.66358200	-0.02470400
O	-1.09018500	2.46533700	-0.91383100
H	-1.53515900	2.82580000	-1.68211100
H	-1.65987300	1.74884500	-0.55324500
O	-0.59475300	0.30642400	2.47929800
H	-0.94589100	0.71154900	3.27331100
H	-1.32137800	0.25638000	1.81681900

O	3.65302300	0.43478700	-0.31750900
H	4.19087200	0.79307900	-1.02786700
H	4.25950300	-0.01297800	0.27769800

$Phe^{+}(H_2O)_3$

N	-2.24799000	0.59483400	0.07902100
H	-2.42939800	0.19647800	1.02381000
C	-0.83918800	0.31543100	-0.32627200
H	-0.66007500	0.78556900	-1.29402000
C	0.11877800	0.87134900	0.74441100
C	-0.68381600	-1.18989600	-0.46466600
H	-0.17399700	0.45295300	1.71209400
H	-0.02883000	1.95443100	0.78078600
O	-1.27258900	-1.98090600	0.22978000
O	0.18230600	-1.50828000	-1.40695000
H	-2.89168300	0.14208600	-0.58962600
H	-2.39905500	1.61694800	0.08941000
O	-3.22784200	-1.16533600	-1.85350400
H	-3.68848600	-1.15020800	-2.69758400
H	-3.28197700	-2.07123100	-1.53080000
O	-2.38375500	-0.77007200	2.49215900
H	-2.79946500	-0.84760500	3.35480500
H	-2.10837600	-1.65068500	2.21028800
H	0.33680600	-2.46502900	-1.39790000
C	1.55637800	0.53516500	0.43550600
C	2.18266900	-0.53302200	1.07512800
C	2.25228100	1.25169100	-0.53751900
C	3.48585600	-0.88709200	0.73893200
H	1.65308800	-1.08555000	1.84575900
C	3.55322700	0.89916700	-0.87483700
H	1.77688600	2.09444900	-1.03086400
C	4.17037900	-0.17416600	-0.23902000
H	3.96922000	-1.71339800	1.24620800
H	4.08792200	1.46386000	-1.62889800
H	5.18591500	-0.44719100	-0.49866600
O	-2.18146600	3.42772900	-0.10677000
H	-2.21657600	4.06305300	0.61506600
H	-2.30860000	3.94039900	-0.91071700

$Phe^{+-}(H_2O)_3$

N	-0.89047400	0.93947600	-0.18276300
H	-1.01126000	1.04418100	0.83915600
C	-0.96088400	-0.51263900	-0.55665600
H	-0.67875500	-0.58165000	-1.60850400

C	-0.00441200	-1.33548400	0.31468300
C	-2.40769200	-1.06474400	-0.37349800
H	-0.06776200	-2.36260600	-0.04953900
H	-0.37219300	-1.32161300	1.34457000
H	-1.67690500	1.44990800	-0.62375300
H	0.00160400	1.35776500	-0.48557000
O	-3.42158600	1.92738200	-0.88121000
H	-4.03648100	2.02322900	-1.61038600
H	-3.66232400	1.10458600	-0.40443100
O	-1.71107400	0.50103100	2.46265300
H	-2.42346100	0.11269100	1.89922000
H	-2.13012300	0.88113200	3.23630500
C	1.41481600	-0.83109700	0.27150700
C	2.25652900	-1.15514800	-0.79566800
C	1.89752000	0.00872500	1.27742600
C	3.55243100	-0.65151200	-0.85694500
H	1.89300700	-1.81281000	-1.57897500
C	3.19175000	0.51899000	1.21825900
H	1.24918700	0.25535700	2.11359300
C	4.02269800	0.19199700	0.14990400
H	4.19811100	-0.92254900	-1.68421400
H	3.55372900	1.16594400	2.00867700
H	5.03441000	0.57777600	0.10733300
O	-3.14591800	-0.38779200	0.41316900
O	-2.64728400	-2.09525000	-0.97662100
O	1.48923600	1.95251500	-1.42645400
H	2.27103500	1.41429900	-1.24729500
H	1.80797600	2.84042000	-1.60322400

$Asn^{+}(H_2O)_3$

N	0.99766900	0.97123300	0.86770700
H	1.86612700	1.36778700	0.43446800
C	1.05590600	-0.51768800	0.92490000
H	1.83303700	-0.78528500	1.64638800
C	-0.27917700	-1.11101400	1.35918000
C	1.54081100	-1.01148900	-0.43698600
H	-0.16241000	-2.19094500	1.47690800
H	-0.58403000	-0.70382700	2.32719700
C	-1.34187600	-0.83061200	0.30337000
O	2.11774300	-0.31729800	-1.22375600
O	-0.99850300	-0.38580300	-0.78669700
O	1.31858800	-2.31120500	-0.57211700
H	0.91240700	1.35743100	1.80902100
H	1.65856300	-2.60501300	-1.43064400

H	0.15549000	1.30436600	0.35632400
H	-3.34446700	-0.79082400	0.00554400
O	3.40455100	1.84757400	-0.10872800
H	3.56628100	1.38023800	-0.93606400
H	4.00108000	2.59980000	-0.07017200
N	-2.61095200	-1.08544400	0.63951100
H	-2.86318000	-1.40170600	1.56166900
O	-1.52217800	2.09431500	0.58414600
H	-2.20062200	1.83044800	-0.06597600
H	-1.78766200	2.95849000	0.90952400
O	-3.23401900	0.99525800	-1.35007700
H	-2.50777700	0.53366300	-1.79331700
H	-3.79329300	1.38694600	-2.02633200

$Asn^{+-}(H_2O)_3$

N	0.84683300	-1.21016500	-0.57052100
C	0.06805800	0.03062300	-0.25463000
H	-0.38280100	0.37229700	-1.19076400
C	-1.03053200	-0.34139200	0.74397300
C	0.97017900	1.18834700	0.26207400
H	-0.60222700	-0.95917400	1.53832100
H	-1.44111700	0.56310700	1.18489600
C	-2.07579400	-1.14015900	-0.00578100
O	2.19349600	0.93627100	0.40155100
O	-1.80400200	-2.24833600	-0.45775700
O	0.36098700	2.24064400	0.46683700
H	1.53478600	-1.03088300	-1.32086700
H	0.17813800	-1.95287700	-0.81904000
N	-3.25907300	-0.52450500	-0.18360500
O	3.00135500	-0.14273900	-1.93255400
H	3.00500000	0.43429500	-1.14375600
H	3.39619900	0.34317100	-2.65788200
H	1.37042600	-1.50140400	0.27581800
O	2.09239300	-1.26977800	1.91682400
H	2.69655300	-1.64472800	2.55935800
H	2.41973900	-0.38746400	1.65803800
O	-2.30158300	2.28506900	-0.16263400
H	-2.63465200	3.15952800	-0.37093500
H	-1.35397300	2.40149700	0.07151800
H	-3.30538100	0.48057500	-0.04293300
H	-3.92763600	-0.96880800	-0.79483300

$Ser^{+}(H_2O)_3$

N	0.40614700	0.60491700	0.72734900
H	-0.16176100	1.47271200	0.69092600
C	0.19493000	-0.14615300	-0.53402400
H	0.59615800	0.46323400	-1.34802800
C	0.91090900	-1.49500300	-0.49243000
C	-1.29759900	-0.34097200	-0.73816200
H	0.46214600	-2.11942100	0.28793000
H	0.78611200	-1.97761000	-1.46460200
O	2.27085800	-1.22384800	-0.20725500
O	-2.13475200	-0.01328600	0.05975300
H	2.74277200	-2.05099700	-0.07292900
O	-1.53984000	-0.93496600	-1.89648800
H	1.40480100	0.87270100	0.78585900
H	-2.49470600	-1.06120600	-2.00752100
H	0.10137600	0.03457400	1.53495200
O	-0.92948700	-1.24860400	2.33575700
H	-0.90261100	-1.68672400	3.19135400
H	-1.85750100	-1.08226500	2.13435200
O	-1.28500400	2.69579700	0.02641500
H	-2.21591800	2.46727200	0.11655300
H	-1.23823500	3.65093700	-0.07388600
O	2.89354300	1.45809300	-0.05574900
H	3.54971200	2.15898000	-0.03207600
H	3.33264900	0.65067600	-0.34611000

$Ser^{+-}(H_2O)_3$

N	0.27784000	0.87013000	0.45283600
H	-0.40036900	1.58937900	0.13803800
C	0.30070200	-0.25613800	-0.53415600
H	0.74990000	0.13320900	-1.44944300
C	1.11979300	-1.41086200	0.00186100
C	-1.14379500	-0.77842200	-0.84967900
H	0.66908800	-1.77628400	0.93132400
H	1.10033700	-2.20010100	-0.75118200
O	2.45816400	-0.96334000	0.25076900
O	-2.06754800	-0.28831900	-0.13061400
H	2.94701200	-1.66433100	0.68839000
O	-1.19361100	-1.61439800	-1.73440700
H	-0.05198600	0.52594900	1.36978700
O	-1.15714000	-0.58605100	2.35549200
H	-1.68561500	-0.63034400	3.15354600
H	-1.76647200	-0.58543700	1.58460900
O	-1.96827400	2.35885400	-0.32117800
H	-2.33590500	1.44991600	-0.33419600

H	-2.34301100	2.83280100	-1.06518500
H	1.20880000	1.29991300	0.52412400
O	2.86678600	1.67237800	-0.29549300
H	3.15532900	0.74926000	-0.25211300
H	3.64079700	2.22469200	-0.41226400

$Thr^{+}(H_2O)_3$

N	0.17584800	0.38059000	1.13339900
H	1.09881100	-0.02260100	1.38858300
C	-0.60502700	-0.67705500	0.43651100
H	-0.58890500	-1.57424600	1.05748600
C	-2.05129000	-0.25426100	0.16641400
C	0.10443500	-0.97916600	-0.87661900
H	-2.52564600	-1.11784400	-0.31078500
C	-2.81468900	0.12858100	1.42525800
O	-1.96608900	0.82790500	-0.75432700
O	0.98659200	-0.30990000	-1.33206100
H	-2.42833700	1.05358600	1.86158500
H	-3.86433600	0.30492900	1.18464000
H	-2.77785200	-0.67213900	2.16747500
H	-2.84487200	1.03976500	-1.08447900
H	-0.29874200	0.68203100	1.98459400
O	-0.41813300	-2.05645700	-1.44466300
H	0.33491500	1.21768700	0.52264100
H	0.03038700	-2.22676800	-2.28670300
O	0.39746100	2.49547300	-0.64182900
H	0.44631500	3.45366200	-0.58222700
H	-0.35441400	2.28064800	-1.20792100
O	2.92326900	0.97070200	0.22242900
H	2.47291100	1.06823500	-0.62720500
O	2.21101500	-1.43568300	1.23688700
H	2.65719800	-2.10696900	1.75891500
H	2.89111300	-0.89114700	0.80905300
H	3.64702500	1.60212800	0.22969000

$Thr^{+-}(H_2O)_3$

N	-0.09590100	0.00065600	-1.10648000
H	-0.85526400	-0.36531700	-1.70675300
C	-0.02538100	-0.85735800	0.13418800
H	-0.34876900	-1.85810900	-0.15982800
C	1.38593900	-0.89848600	0.70985400
C	-1.06307900	-0.24295100	1.13117100
H	1.30626800	-1.46830700	1.64171500

C	2.41111300	-1.56348200	-0.19216700
O	1.82596300	0.42100000	1.01139600
O	-2.24325400	-0.20660900	0.69664000
H	2.54715900	-1.02483100	-1.13277500
H	3.37664300	-1.58488200	0.31475200
H	2.11161500	-2.59026900	-0.41140000
H	1.19616400	0.73954800	1.68239300
H	0.79282100	0.05577600	-1.61381400
O	-0.61373700	0.21926800	2.18250500
H	-0.35254700	0.97565200	-0.85628500
O	-2.40460000	-1.33081100	-1.69295300
H	-2.59529600	-0.99843100	-0.78176400
H	-3.23590300	-1.40662100	-2.16282600
O	-1.48991800	2.29370200	-0.21768600
H	-2.09429000	1.69417500	0.25370800
H	-1.25381100	2.97854800	0.41176700
O	2.24201300	1.45925500	-1.49235900
H	2.33834800	1.35627300	-0.52986800
H	2.95487500	2.01941400	-1.80228500

$Val^{+}(H_2O)_3$

N	-0.09418300	1.19804400	-0.10289100
H	-0.34702600	1.22418300	0.90456200
C	0.24248600	-0.18237800	-0.55616400
H	0.35756100	-0.14895200	-1.64197700
C	1.55010500	-0.67564400	0.10178200
C	-0.95759900	-1.05379800	-0.22816400
O	-1.85786800	-0.70891500	0.49410000
O	-0.88182400	-2.23706700	-0.81735500
H	-0.92763300	1.51928000	-0.62318700
H	0.70109800	1.83290100	-0.28396600
O	-2.38711600	1.15862400	-1.68998700
H	-2.75628900	1.59549900	-2.46305900
H	-3.13033900	0.77377200	-1.21361300
O	-1.20428100	1.21225400	2.46384800
H	-1.32488700	1.67842800	3.29503600
H	-1.87357000	0.52095800	2.41265600
H	-1.65090200	-2.77049400	-0.56415300
H	2.23928700	0.17354000	0.02756600
C	2.16219200	-1.84137800	-0.67550800
C	1.34854900	-1.02936400	1.57621100
H	2.30882500	-1.59102800	-1.72845200
H	3.13641400	-2.08544800	-0.24942500
H	1.53670300	-2.73285100	-0.61944800

H	0.89662200	-0.21872600	2.15292500
H	0.71145300	-1.91379600	1.67819400
H	2.31021300	-1.26778900	2.03233300
O	2.22092900	2.75513000	-0.70706300
H	2.51075700	3.04634700	-1.57693700
H	2.76788000	3.23303400	-0.07610300

$Val^{+-}(H_2O)_3$

N	-0.31670300	1.18403100	0.30735400
H	-0.73255600	0.81740300	1.18258800
C	0.40959300	0.11119500	-0.45436200
H	0.78856300	0.59254100	-1.35856300
C	1.58383300	-0.41896500	0.38780600
C	-0.57894300	-1.01912100	-0.87690000
H	2.02923000	0.44826900	0.89602000
O	-1.72649800	-0.97455900	-0.33103800
O	-0.13202200	-1.82538000	-1.67629600
H	-1.11737100	1.52801300	-0.25163500
H	0.33203800	1.95350700	0.49777700
O	-2.75694200	1.36507400	-1.05250000
H	-3.20940800	1.50118700	-1.88634400
H	-2.65383600	0.39635400	-0.92686200
O	-1.90528200	-0.18142200	2.21438300
H	-2.78045000	0.01561900	2.55272500
H	-2.02636000	-0.67772200	1.37450700
C	2.64858700	-1.04501600	-0.51360100
C	1.12124100	-1.41075300	1.45797200
H	3.02549700	-0.32597000	-1.24778700
H	3.49095100	-1.39526100	0.08730600
H	2.22481300	-1.88797700	-1.06117400
H	0.70218900	-2.30265700	0.98435700
H	1.97116200	-1.71876900	2.07090400
H	0.36130900	-0.99279900	2.12277300
O	1.98608900	2.89345800	-0.00989600
H	2.18610500	3.82325700	-0.14331300
H	2.79642300	2.41538400	-0.20747900

$Ile^{+}(H_2O)_3$

N	0.38615600	-1.86477200	-0.63870500
H	0.62306200	-2.08403500	0.35281600
C	-0.29427600	-0.53824100	-0.77713000
H	-0.37371500	-0.32859800	-1.84645300
C	-1.69524500	-0.56493700	-0.13046600

C	0.64244500	0.49026800	-0.15448500
H	-2.14048900	-1.52597100	-0.42574200
O	1.60160000	0.17215000	0.51683200
O	0.27973400	1.71332900	-0.42538900
H	1.28647300	-1.83149800	-1.15585200
H	-0.20074000	-2.60943200	-1.01457300
O	2.66071500	-0.98161400	-1.90301600
H	3.24277800	-1.14322400	-2.65095300
H	3.15469400	-0.45380500	-1.26621800
O	1.40662200	-2.26975100	1.89890200
H	1.61639400	-2.88237400	2.60839200
H	1.88495500	-1.44791800	2.05556500
H	0.90049400	2.36557200	0.00088400
C	-1.61113300	-0.51161900	1.39663200
C	-2.59083500	0.53706000	-0.71419100
H	-1.31042100	0.48795700	1.72656800
H	-2.58389800	-0.72643200	1.83773200
H	-0.89913100	-1.23310300	1.80533300
H	-2.58804900	0.44908700	-1.80567400
H	-2.16595700	1.51507600	-0.47666700
C	-4.02858200	0.45529300	-0.20531000
H	-4.44806300	-0.54280400	-0.35843200
H	-4.09695900	0.69341700	0.85728400
H	-4.65935400	1.16597400	-0.73989900
O	1.93583800	3.41969400	0.70981200
H	2.53584200	3.16790500	1.41681600
H	1.90868200	4.38019200	0.68257800

Ile^{+-} $(H_2O)_3$

N	0.89939000	-1.78317500	0.06003200
H	1.19355100	-1.39500200	0.98017700
C	-0.11793100	-0.90352200	-0.61906300
H	-0.29726800	-1.34309000	-1.60248500
C	-1.42197700	-0.87552700	0.19610400
C	0.48366100	0.51437700	-0.81497600
H	-1.63653300	-1.91580700	0.48979500
O	1.52922100	0.77363200	-0.13527400
O	-0.12501500	1.24373200	-1.58348800
H	1.76862200	-1.81548100	-0.50571300
H	0.53425900	-2.72465600	0.19669700
O	3.23769500	-1.02077000	-1.18813800
H	3.74137100	-0.91379600	-1.99686900
H	2.90290700	-0.14034000	-0.92642700
O	1.97341800	-0.39706200	2.24714100

H	2.84335400	-0.38580300	2.65052500
H	1.95472800	0.30589100	1.56778400
C	-1.27717800	-0.02596800	1.46225700
C	-2.58883300	-0.41001200	-0.68593800
H	-1.13162500	1.02860600	1.20378300
H	-2.17434100	-0.10583000	2.07712900
H	-0.43273500	-0.33468200	2.08330500
H	-2.61316300	-1.03040900	-1.58869500
H	-2.39279700	0.61146800	-1.01904500
C	-3.94048900	-0.49307600	0.02008800
H	-4.10651600	-1.48745400	0.44624100
H	-4.02001600	0.23721300	0.82690700
H	-4.75072300	-0.29193200	-0.68269900
O	0.22574200	3.33736600	0.41609100
H	0.95571000	2.70614600	0.41090600
H	-0.18651100	3.14438400	-0.43305000

$Leu^{+}(H_2O)_3$

N	-1.19944300	1.06345700	-0.03187900
H	-1.39739800	1.02671300	0.98887700
C	-0.16591000	0.04532000	-0.38034300
H	0.02355900	0.11401900	-1.45250200
C	1.10809800	0.32787300	0.42856300
C	-0.75737900	-1.31728200	-0.06998400
H	1.39315800	1.36349500	0.20653600
O	-1.66282800	-1.49341400	0.70556700
O	-0.14686100	-2.28175900	-0.74072000
H	-2.07430600	0.85043500	-0.53876200
H	-0.85538600	2.00348200	-0.28929000
O	-3.15852900	-0.30910900	-1.47351400
O	-1.58795100	0.52145000	2.66947400
H	-1.79589700	0.89063000	3.53179500
H	-1.90491300	-0.38879800	2.65565800
H	-0.52124300	-3.13856100	-0.48480200
C	2.30658300	-0.58104000	0.12592100
H	2.05764300	-1.60434100	0.42471700
C	3.49503500	-0.11481600	0.96809000
H	3.80692400	0.89082600	0.67049900
H	3.25094300	-0.09491700	2.03276100
H	4.34734900	-0.78187300	0.83031900
H	0.85279100	0.27764700	1.49300000
C	2.66229700	-0.58051600	-1.36117500
H	2.81137500	0.44309300	-1.72166700
H	3.59289200	-1.12539300	-1.52828500

H	1.89436200	-1.05870600	-1.97292800
H	-3.54256100	-1.01012200	-0.93603500
H	-3.73483400	-0.20028000	-2.23553600
O	0.03978400	3.48661000	-0.86753400
H	0.35051600	4.19833700	-0.29953300
H	0.07986700	3.83265300	-1.76428000

$Leu^{+-}(H_2O)_3$

N	-1.12931000	1.11684300	0.47614600
H	-1.38720000	0.63293600	1.35683200
C	-0.12734900	0.29441100	-0.28595300
H	0.18507300	0.90596400	-1.13265300
C	1.04498400	-0.01887800	0.64518300
C	-0.79071500	-0.99810000	-0.84225900
H	1.41954000	0.92248300	1.07374200
O	-1.81425800	-1.40319400	-0.20404600
O	-0.24739800	-1.48019600	-1.82353200
H	-2.00138400	1.21685600	-0.07323200
H	-0.71982200	2.03600900	0.66698300
O	-3.52764700	0.55062000	-0.84553300
H	-3.97814900	0.56396700	-1.69158100
H	-3.16466300	-0.35252100	-0.72623400
O	-1.75047900	-0.82981700	2.37518000
H	-2.44823100	-1.12601200	2.96152000
H	-1.87220300	-1.28520700	1.50789200
C	2.21332200	-0.75100800	-0.02339000
H	1.84517900	-1.71059800	-0.39642200
C	3.30738500	-1.00348300	1.01378400
H	3.71132600	-0.05636000	1.38814700
H	2.92330800	-1.56600700	1.86820700
H	4.13321800	-1.57030100	0.57829100
H	0.66626200	-0.61663700	1.48211600
C	2.76586300	0.03198000	-1.21410200
H	3.04778600	1.04982000	-0.91044700
H	3.66692200	-0.44581600	-1.60530400
H	2.04119300	0.08306500	-2.02852400
O	0.71853400	3.28750500	0.10050100
H	0.82371100	4.24191400	0.09484000
H	1.50234100	2.92966000	-0.32733100

$Pro^{+}(H_2O)_3$

N	0.68989900	0.85741500	-0.10850100
C	-0.24528800	1.44286400	-1.14732400

C	0.00172400	-0.31629200	0.53106600
H	0.13256100	1.11817900	-2.11668200
H	-0.20564400	2.52867900	-1.08614000
C	-1.59884400	0.82241300	-0.82405400
C	-1.22707700	-0.58127700	-0.35065200
H	-0.29984400	-0.02114200	1.53791700
C	0.95237000	-1.49066700	0.61321800
H	-2.26671900	0.81158100	-1.68282900
H	-2.10341300	1.36585000	-0.02166100
H	-0.94564300	-1.21160800	-1.19990100
H	-2.02806800	-1.06627600	0.20210500
O	2.03176800	-1.52331100	0.08694800
O	0.41393600	-2.47864300	1.31177300
H	1.56649700	0.56706700	-0.58122400
H	0.91573700	1.55247200	0.61928000
H	1.02269300	-3.23270800	1.32872700
O	2.62334400	0.20321400	-2.01550500
H	3.18516300	0.59995200	-2.68638700
H	3.02319700	-0.63805200	-1.76937100
O	0.96221800	2.55761800	2.12732000
H	0.35934900	3.24996900	2.41430700
H	1.75092500	2.65679800	2.66954600
O	-4.33271100	-0.34061600	-0.19158100
H	-4.99379300	0.08848100	0.35800400
H	-4.82803700	-0.97949300	-0.71135100

$Pro^{+-}(H_2O)_3$

N	-0.72334400	0.75199900	-0.55541800
C	-2.19223700	1.06736600	-0.62451900
C	-0.39588000	0.25635400	0.82737900
H	-2.60789700	0.45858900	-1.42536600
H	-2.32572400	2.12253400	-0.85522700
C	-2.74728300	0.66165800	0.74949600
C	-1.72112600	-0.34630800	1.27930600
H	-0.12139200	1.12224400	1.43092000
C	0.80405700	-0.71830400	0.75978400
H	-3.75024900	0.24509000	0.66287200
H	-2.79410800	1.53067600	1.40999900
H	-1.86127900	-1.32026000	0.80234700
H	-1.75149900	-0.47073200	2.36041300
O	0.92124000	-1.33776700	-0.33879000
O	1.52541300	-0.75933600	1.75067400
H	-0.50839600	-0.02579300	-1.19580300
H	-0.07085300	1.51547800	-0.79435400

O	3.38761200	-0.02448900	-0.32910900
H	2.81079700	-0.73571400	-0.65367200
O	-1.31937100	-1.78897600	-1.71930200
H	-0.46027400	-1.95437500	-1.27641400
H	-1.39065100	-2.41493100	-2.44181600
H	3.35586500	-0.18368500	0.62426000
O	1.67738200	2.05017300	-0.75963400
H	2.35315300	1.34455600	-0.61860600
H	2.16250900	2.86090000	-0.92102300

$Sar^{+}(H_2O)_3$

N	0.35187900	1.01744200	-0.39596600
H	0.93815200	0.55552400	0.31782300
C	-0.37671300	-0.01302700	-1.16949400
H	-1.15992600	0.46850500	-1.75749300
C	-0.99682200	-1.00594300	-0.21301100
O	-0.93336900	-0.91009800	0.98656900
O	-1.61385600	-1.97030500	-0.86844200
H	-0.35937000	1.56328500	0.12083200
O	-2.05800200	1.77761600	0.74053500
H	-2.65140400	2.53018400	0.82135600
H	-2.30391300	1.15548100	1.43339000
O	2.21850600	-1.09141400	-0.46553700
H	2.83167100	-1.68585400	-0.90570700
H	2.42129900	-1.13097500	0.47813800
H	-2.00402900	-2.59846900	-0.24154800
H	0.32212400	-0.53091900	-1.82376800
C	1.20439900	1.88937400	-1.24769300
H	0.58432700	2.35667400	-2.01061800
H	1.66137700	2.65031600	-0.61889900
H	1.97199700	1.26470000	-1.69954500
O	1.57138600	-0.12558000	2.02054800
H	0.77022400	-0.56348400	2.33346200
H	2.05181500	0.17876800	2.79613800

$Sar^{+-}(H_2O)_3$

N	-1.35310300	0.58539300	-0.01989800
H	-1.59270700	-0.21238800	-0.63595800
C	-0.71851800	0.03405800	1.21357300
H	-0.51589600	0.85769100	1.89629500
C	0.60594200	-0.67827000	0.84034700
O	0.59437100	-1.25300400	-0.28851700
O	1.52780100	-0.57768200	1.64135800

H	-0.62004500	1.14657600	-0.50400300
O	0.87974800	1.90434900	-0.90475200
H	1.68075000	1.32147900	-0.89270400
H	1.17206900	2.77533200	-1.17751900
O	-1.81460300	-1.92045000	-1.09222000
H	-1.98808600	-2.47603600	-1.85319300
H	-0.84670000	-1.95223500	-0.90236400
H	-1.41949000	-0.66947300	1.66741200
C	-2.55917700	1.39767000	0.23916100
H	-2.29052400	2.24432500	0.86901600
H	-2.96217900	1.75452100	-0.70719600
H	-3.29937700	0.77976100	0.74549900
O	2.91001100	0.14312200	-0.77757400
H	3.09096400	0.05573800	0.16813200
H	2.31483400	-0.61446700	-0.91897300

$DMGly^{+}(H_2O)_3$

N	-1.52645100	-0.57552300	-0.13938300
C	-0.34099300	-1.16586300	0.53719200
H	-0.42522800	-0.98860900	1.60769600
C	0.93923900	-0.50853300	0.04876100
O	0.95095400	0.38194600	-0.77012600
O	1.97860600	-1.03471800	0.63095900
H	-1.37351600	0.44547700	-0.19697700
O	-1.11900200	2.18808400	-0.93497800
H	-1.51263200	2.88788600	-1.46343200
H	-0.23525300	2.01094400	-1.28426400
H	2.81859600	-0.59243200	0.32584400
H	-0.31834700	-2.24058200	0.34632600
C	-2.76728900	-0.79737200	0.65694800
C	-1.67553300	-1.06988900	-1.53888800
H	-2.64089500	-0.30590600	1.61879000
H	-3.60595000	-0.36008400	0.11808400
H	-2.91804400	-1.86989900	0.77782400
H	-1.90515800	-2.13466100	-1.50775400
H	-2.48958500	-0.52381500	-2.01166700
H	-0.74631100	-0.88813200	-2.07373100
O	-0.82370700	1.44561300	1.70836600
H	-0.62036000	1.81249400	2.57254600
H	-0.85628600	2.18872600	1.09186800
O	4.17551300	0.15452300	-0.17736900
H	4.20023700	0.76861100	-0.91587700
H	5.08244100	-0.01499900	0.09150200

DMGly $^{+-}$ $(H_2O)_3$

N	1.15082800	0.86870000	-0.10948000
H	1.99948400	0.26928100	-0.07849300
C	0.05573200	0.04670000	-0.71747700
H	-0.83295800	0.67283700	-0.78708800
C	-0.21920000	-1.24576700	0.10176400
O	0.77282600	-1.75748100	0.65783500
O	-1.39866600	-1.62954900	0.09982400
O	3.09849000	-1.05507500	-0.32202000
H	3.93804400	-1.41680900	-0.03496000
H	2.37196100	-1.59086300	0.07796100
H	0.38640200	-0.23928500	-1.71867400
C	1.46164800	2.04434000	-0.95698100
C	0.82045900	1.27687900	1.28641700
H	0.57932900	2.68220100	-1.00430000
H	2.29458400	2.58971300	-0.51561600
H	1.72996400	1.69844700	-1.95363000
H	0.75270500	0.37370000	1.88917900
H	1.61934000	1.91901400	1.65488800
H	-0.14118100	1.79029100	1.28144800
O	-2.34018400	1.03240500	1.28258800
H	-2.86700700	0.97891100	0.47144400
H	-2.22119600	0.10190900	1.50630000
O	-3.11874800	-0.02390400	-1.20217000
H	-3.89374700	-0.41150400	-1.61157100
H	-2.59309600	-0.76282900	-0.82132800

Bet^{+} $(H_2O)_3$

N	-0.60706600	-0.97103600	0.07625500
C	-0.04112600	0.28632300	-0.51306100
H	0.47650300	0.02442500	-1.43677200
C	0.95731200	1.00796100	0.37014700
O	1.37971900	0.62705600	1.42525000
O	1.28306800	2.15597300	-0.21105100
O	2.87870900	-0.46073700	-0.97975500
H	3.41818400	-0.33703300	-1.76620700
H	3.50739800	-0.55404300	-0.25727900
O	-3.05157600	1.56070500	-0.46101400
H	-3.86250400	1.51144300	-0.97672500
H	-3.05585000	2.44876200	-0.09004200
H	1.94727900	2.60722600	0.33063400
H	-0.88016100	0.94802000	-0.73889300
C	0.45943800	-1.99799000	0.32842400

C	-1.57665300	-1.51844300	-0.92712500
C	-1.35538300	-0.68044400	1.34669300
H	1.10672800	-1.64091900	1.12383500
H	-0.03582400	-2.92304700	0.62012600
H	1.03277600	-2.13212700	-0.58709100
H	-1.03851500	-1.74598400	-1.84617800
H	-2.01842200	-2.42547000	-0.51809600
H	-2.34309300	-0.76609800	-1.10443500
H	-2.13159000	0.04945000	1.11840800
H	-1.79963400	-1.61344000	1.69102200
H	-0.65469700	-0.30232600	2.08599300
O	-1.35728635	-0.39351878	-3.04397466
H	-0.39728635	-0.39351878	-3.04397466
H	-1.67774094	0.51141706	-3.04397466

Bet $^{+-}$ $(H_2O)_3$

N	-0.60850400	-0.04561200	0.27935500
C	0.82502000	0.06023500	0.76003700
H	0.88499200	0.97995200	1.33926800
C	1.81107100	0.10589600	-0.44645200
O	2.23478200	1.23488900	-0.74572100
O	2.02881800	-0.98851600	-1.00188700
O	0.90621100	3.17075400	0.55192400
H	1.33553300	4.02534400	0.61025300
H	1.51848500	2.58440300	0.04613100
O	1.45928200	-3.09208700	0.60637100
H	1.76434700	-2.42676800	-0.05015300
H	2.19343700	-3.69585100	0.72760600
H	1.00571600	-0.81746300	1.38259600
C	-0.88076400	0.94074500	-0.81451400
C	-1.50769300	0.25909900	1.42952900
C	-0.90638400	-1.42346200	-0.22345800
H	-0.25416200	0.68848200	-1.66843800
H	-1.93545500	0.85263400	-1.07239500
H	-0.63059800	1.93795900	-0.45283400
H	-1.31650300	1.28471100	1.74439600
H	-2.53993300	0.13751800	1.10248700
H	-1.27483700	-0.43316700	2.23799900
H	-0.71646400	-2.13763400	0.57602800
H	-1.94834700	-1.43372800	-0.54079800
H	-0.23327700	-1.63760400	-1.05045100
O	3.81268921	-0.01808787	-2.24072441
H	3.41077586	0.85372957	-2.24072441
H	3.25862982	-0.80206377	-2.24072441

H_3O^+

O	0.00000000	0.00000000	0.00000000
H	0.00000000	0.97471500	0.00000000
H	0.84412800	-0.48735800	0.00000000
H	-0.84412800	-0.48735800	0.00000000

H_2O

O	0.00000000	0.00000000	0.11657000
H	0.00000000	0.76160200	-0.46627900
H	0.00000000	-0.76160200	-0.46627900