Supporting Information

Microsolvation of Zn cations: Infrared spectroscopy of hydrated $Zn^+(H_2O)_n$ complexes (n = 2–35)

Ethan M. Cunningham, Thomas Taxer, Jakob Heller, Milan Ončák, Christian van der Linde, and Martin K. Beyer*

Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

Corresponding author: martin.beyer@uibk.ac.at

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Calculating IRMPD cross sections

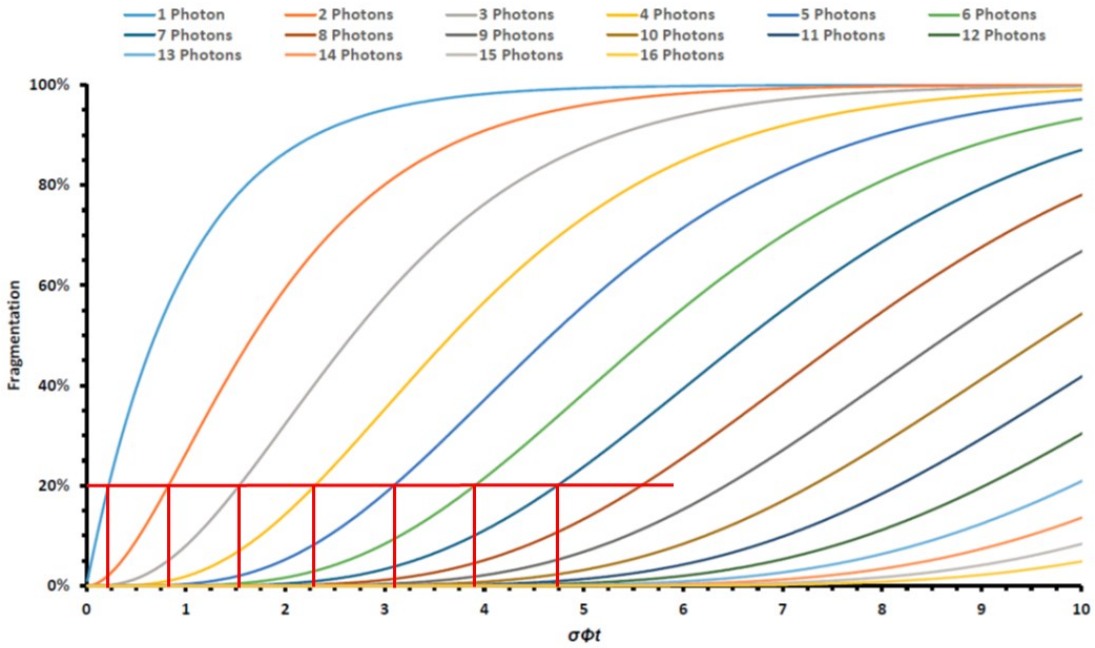

Figure S1. Quantitative analysis of multiphoton absorption, each curve representing *k* photons (*k* = 1–16) with the fragmentation yield (%) and $\sigma\Phi t$.

As outlined in previous publications,[1,2] infrared multi-photon photodissociation cross sections are calculated assuming consecutive first-order reactions, the kinetics of photon absorption is shown in Figure S1. Using Figure S1, along with the fragmentation yield after absorption of the k^{th} photon, the value of $\sigma\Phi t$ can be readily obtained. By way of example, the values of $\sigma\Phi t$ are shown for 1-7 photons, assuming a 20% fragmentation yield. The photon flux, Φ, is measured using a power meter, t is controlled using the LabView software, thus the cross section, σ, can be calculated from $\sigma\Phi t$.

The number of photons required to dissociate a water molecule ranges from one to two, details of which is found in previous publications.[1,2] For all cluster sizes, photodissociation leading to loss of water molecules was found to be the only photofragment channel. To account for laser energy and irradiation time, single-photon cross sections, σ, are calculated using a modified Beer-Lambert equation, details are outlined in the experimental section of the main article.

Calculated H_2O Binding Energies

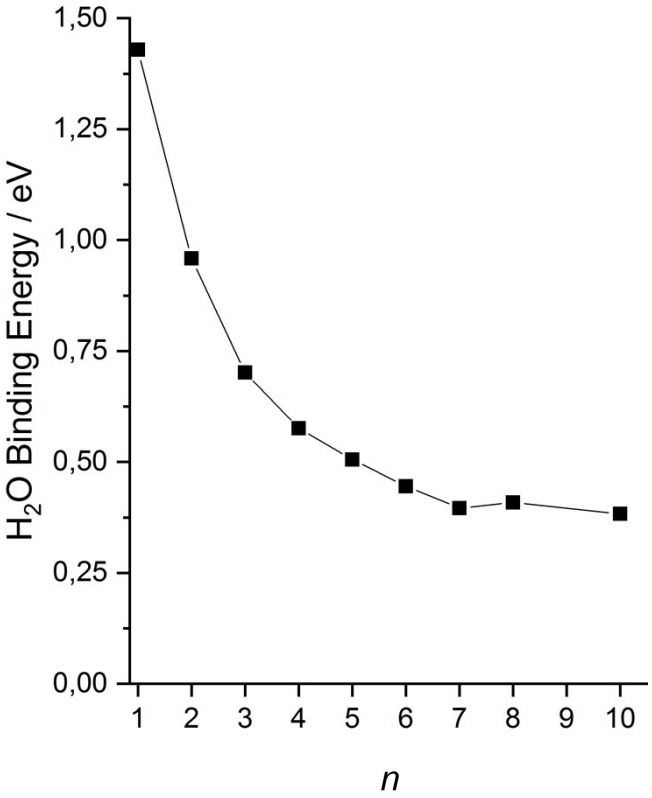

Figure S2. Ligand binding energies of $Zn^+(H_2O)_n$ clusters (n = 1–10) calculated at the B3LYP/aug-cc-pVDZ level of theory. Binding energies are calculated: $E[Zn^+(H_2O)_n] - E[Zn^+(H_2O)_{n-1}] - E[(H_2O)]$ including zero-point correction, assuming a coordination number of 3 for all clusters where $n \geq 3$.

Calculated Structures

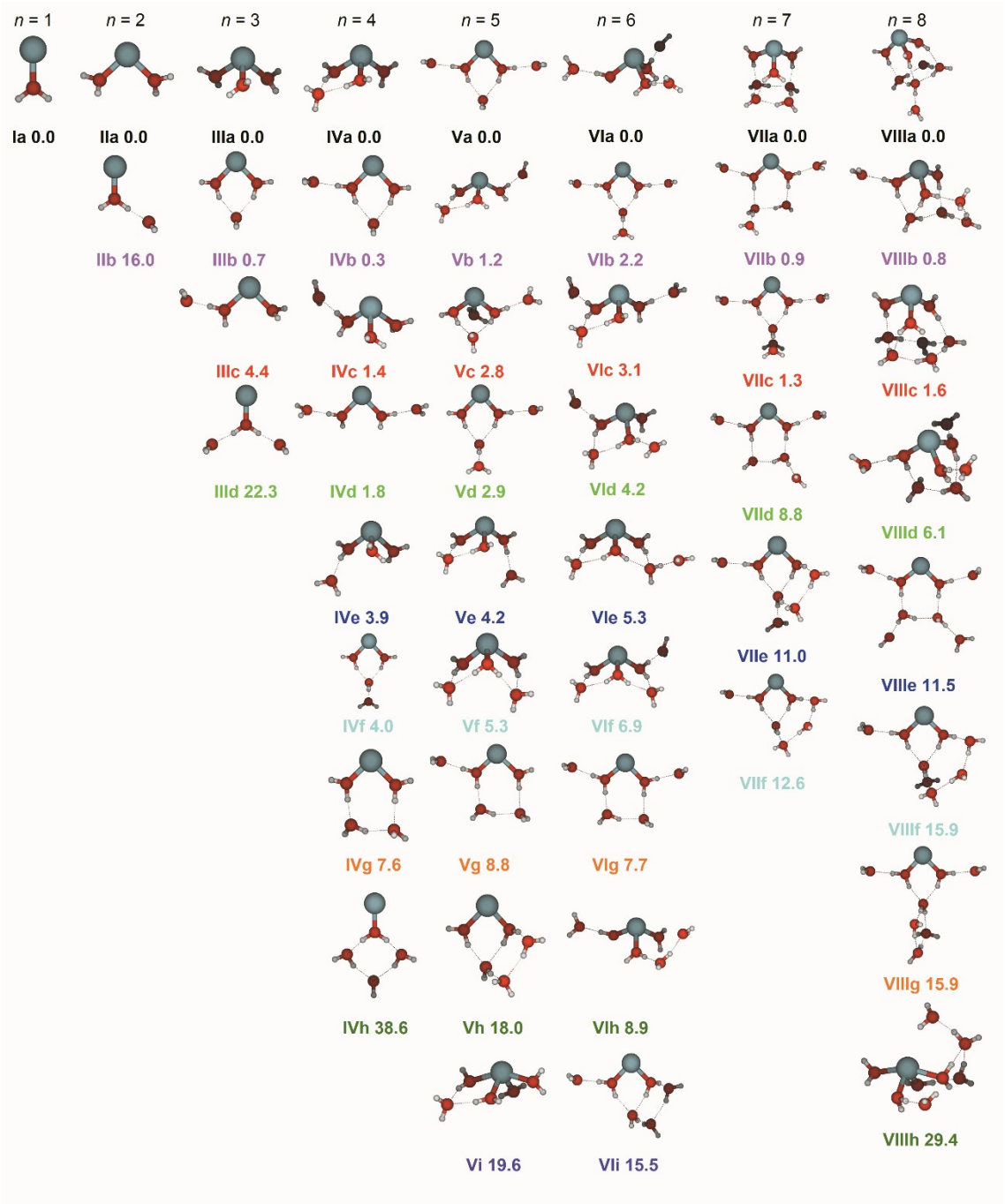

Figure S3. Low-lying isomers of $Zn^+(H_2O)_n$ clusters (n = 1–8) calculated at the B3LYP/aug-cc-pVDZ level of theory along with relative energy given in kJ mol^{-1} inclusive of zero-point energy.

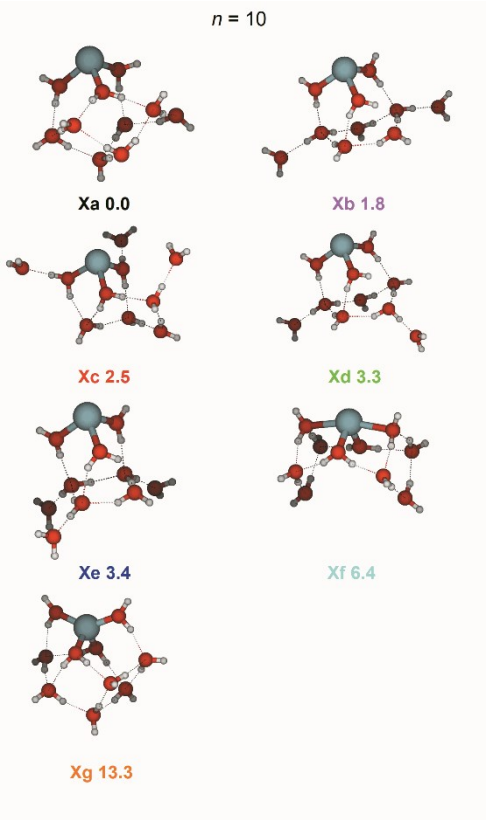

Figure S4. Low-lying isomers of the $Zn^{+}(H_2O)_{10}$ cluster calculated at the B3LYP/aug-cc-pVDZ level of theory along with relative energy given in kJ mol^{-1} inclusive of zero-point energy.

Cartesian coordinates (in Å) and electronic energies (in Hartree), inclusive of zero-point energy, for $Zn^+(H_2O)_n$ clusters (n = 1-10) optimised at the B3LYP/aug-cc-pVDZ level of theory.

Ia

-1855.620360
H 0.785918 -2.084069 0.000000
O 0.000007 -1.513340 0.000000
H -0.786192 -2.083688 0.000000
Zn 0.000007 0.542483 0.000000

IIa

-1932.078999
O -1.553704 0.849674 0.021610
Zn -0.000310 -0.599483 0.000054
O 1.554253 0.849097 -0.021616
H -2.455405 0.622010 0.297306
H -1.629112 1.578635 -0.614351
H 1.635801 1.571910 0.620601
H 2.453633 0.621769 -0.305117

IIb

-1932.072916
O 0.539390 0.812983 0.000074
Zn -1.189757 -0.164186 -0.000003
O 2.815099 -0.358396 -0.000045
H 0.621871 1.777652 -0.000495
H 1.463499 0.388917 -0.000098
H 3.386043 -0.439165 -0.776133
H 3.385391 -0.438534 0.776590

IIIa

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Zn 0.000517 0.000363 -0.651096
O -1.015158 1.442259 0.625994
H 2.643860 -0.012562 0.275392
H 1.838957 0.911063 1.230142
H -1.311688 2.295484 0.274916
H -1.711014 1.135615 1.227536
O -0.743077 -1.600000 0.625110
H -1.331098 -2.284999 0.272710
H -0.131778 -2.047139 1.230480

IIIb

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O 0.311617 1.440846 -0.000754
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O 0.312155 -1.440163 -0.001258
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H 3.277210 0.001875 -0.767727
H 1.262073 -1.196532 -0.001847
H 0.219090 -2.402172 0.000341
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H 1.262088 1.199417 0.000017

IIIc

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H -1.789142 1.947367 0.384361
H -2.980093 0.943996 0.529860
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H 3.756679 0.814502 0.806375
H 3.847727 -0.560447 0.099780

IIId

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H -2.231673 -2.654316 -0.773732
H -2.232261 2.654040 -0.773610
H -2.231264 2.654537 0.773849

IVa

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O 0.605573 -1.449000 0.226681
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H 3.516741 0.052349 1.104774
H 1.534654 1.202225 0.154413
H 0.550305 2.373998 -0.203991
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H 1.552994 -1.204694 0.229009

O -2.057051 0.036644 1.142490
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H -1.797779 0.367584 2.014868

IVb

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O -3.460918 0.309312 -0.000008
O 0.961840 2.619948 0.000064
H 1.941087 1.071119 0.000091
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H -0.491830 1.284588 0.000036
H -1.816093 0.352157 -0.000036
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H -4.028913 0.205760 0.773843
H 1.033001 3.203937 0.768897
H 1.033015 3.203717 -0.768935

IVc

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H -1.704703 2.423951 0.079986
O 1.023342 -0.283043 0.754093
H 1.976959 -0.209769 0.478598
H 0.960156 -1.022183 1.375154
O 3.552995 -0.015136 0.004641
H 4.014817 -0.521452 -0.675640
H 4.231970 0.465432 0.495004

IVd

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Zn 0.000000 -0.601184 0.000308
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H 2.478910 0.530851 -0.110497
H 4.623836 0.395124 0.776128
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IVe

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Zn 0.787075 -0.044180 -0.642839
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O 1.791844 -0.589694 1.236693
O -3.286375 0.061052 0.292720
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H 1.370930 -1.259900 1.796173
H 2.743973 -0.765142 1.264423
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IVf

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Vb

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Vd

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Ve

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H 3.328534 2.334780 0.773786
H 3.329381 2.336229 -0.768831

Vf

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H 2.249707 -0.033736 0.706719
H 2.294712 -1.575210 1.013959

Vg

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Vh

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H 4.315020 0.472825 -0.079321

Vi

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VIa

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H 3.534356 -2.911328 -1.034392
H -4.288261 -1.604580 -1.034694
H -4.885628 -0.891451 0.199728
O 1.036411 4.082453 -0.219609
H 1.670940 4.676577 0.199842
H 0.754915 4.515811 -1.034755

VIb

-2237.854881
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O 1.443031 -0.261520 0.143164
Zn -0.000733 -1.634937 -0.260139
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VIc

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O 1.238939 0.622038 0.465298
Zn -0.322516 -0.124181 -0.768213
O -1.694293 0.047954 0.812243
O 0.372648 -2.136164 -0.315231
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H 1.971581 0.006525 0.648237
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H -2.663223 0.204390 0.688440
H 2.465493 3.453591 -0.886643
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VId

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Zn -0.015479 -0.889791 -0.419531
O 0.142852 -2.045054 1.444623
O -1.500715 0.433807 0.217213
O 3.913950 0.505642 -0.831420
O -4.041170 0.400424 -0.685772
H 2.367523 0.433827 -0.087342
H 1.192992 1.320430 0.503403
H -2.424188 0.413287 -0.130217
H -1.248272 1.359260 0.385210
H 0.034839 3.573740 0.226226
H -0.056596 3.165439 1.704484
H 0.885626 -1.821625 2.024330
H 0.064130 -3.009243 1.449369
H -4.328199 0.290863 -1.600888
H -4.798169 0.161344 -0.136440
H 4.103333 0.336295 -1.762762
H 4.763924 0.474063 -0.374931

VIe

-2237.853713
O -2.510975 2.426791 0.089126
O -2.562714 -0.353660 0.540174
Zn -0.799043 -1.028752 -0.538732
O -0.078709 0.984312 -0.524685
O 0.563741 -1.452725 1.068689
O 2.272940 0.680270 0.928535
O 4.538760 0.549647 -0.534689
H 0.754538 1.123853 -0.026023
H -0.710594 1.686883 -0.289610
H -3.381202 -0.866240 0.496995
H -2.794207 0.589820 0.420805
H -2.951446 2.843000 -0.665350
H -2.656043 3.030522 0.831024
H 5.310690 -0.005395 -0.368158
H 4.791040 1.154836 -1.243075
H 1.324750 -0.829121 1.124477
H 0.898681 -2.349327 1.201060
H 2.489368 1.163774 1.736093

H 3.111354 0.642884 0.406511

VIf

-2237.853075
O 0.755762 2.956128 0.224816
O 1.493763 0.176491 0.462878
Zn -0.022870 -0.764578 -0.636160
O -1.369250 -1.478773 0.941479
O -1.168258 1.061110 -0.655869
H 1.124297 3.533882 -0.458163
H 0.716253 3.501417 1.022637
H -0.720496 1.861495 -0.321423
H -2.068120 1.025769 -0.284262
H 2.425099 -0.148970 0.419353
H 1.507389 1.150231 0.440790
H -2.280148 -1.128675 0.875699
H -1.436052 -2.428445 1.110110
O -3.651818 0.131054 0.465277
H -4.137131 0.514201 1.209261
H -4.329896 -0.106314 -0.183111
O 4.046610 -0.692175 0.374874
H 4.498252 -1.053297 -0.398174
H 4.532188 -1.014639 1.144446

VIg

-2237.852788
O 1.591899 0.103951 -0.153812
Zn 0.164046 -1.293491 0.031453
O -1.511398 -0.111429 -0.041807
O 4.209742 -0.507436 -0.119492
O -3.989320 -1.134008 0.106054
H 1.465177 1.059535 0.082529
H 2.552080 -0.122735 -0.128444
H -1.585098 0.857233 -0.156521
H -2.419422 -0.498613 0.011461
H -4.423512 -1.608965 -0.613992
H -4.387941 -1.463846 0.921470
H 4.757691 -0.642235 -0.902552
H 4.725968 -0.826874 0.630858
O -1.713104 2.719109 -0.343372
H -2.331292 3.143629 0.268181
H -1.966197 3.036702 -1.221550
O 1.026668 2.624063 0.489105
H 0.159710 2.929236 0.172167
H 1.615556 3.387663 0.499395

VIh

-2237.852307
O -0.585255 -2.344610 0.520944
Zn -0.824642 -0.471861 -0.640463
O 5.509171 0.528922 0.513636
O -4.239127 1.805747 0.180154
O -2.199423 0.201015 0.833069
O 0.789190 0.251316 0.482220
O 3.051706 0.862887 -0.633485
H 1.661192 0.509880 0.053418
H 0.574373 0.934560 1.131629
H -4.878863 1.682843 -0.532103
H -0.729570 -3.216050 0.125251
H -4.520012 2.590282 0.667237
H 0.266527 -2.386469 0.981297
H -2.541305 -0.474969 1.434494
H 5.970234 1.194293 1.039307
H -2.963121 0.783254 0.588547
H 6.190412 -0.076991 0.196661
H 3.943090 0.744877 -0.237408
H 3.156193 1.428117 -1.406762

VIi

-2237.849806
O -0.806178 -1.070998 0.830609
Zn 1.019231 -1.403233 -0.044689
O 1.469826 0.605604 0.001635
O -3.017583 -1.110221 -0.658531
O -0.926509 1.703702 1.052825
O -3.324286 1.840665 -0.516338
H -0.904281 -0.143088 1.132299
H -1.633768 -1.257552 0.315385
H -1.725704 1.921023 0.531813
H -0.949860 2.269777 1.835196
H -3.756741 -1.727591 -0.717711
H -3.388267 -0.212844 -0.687377
H -3.277953 2.266138 -1.384400
H -4.113014 2.215470 -0.099147
H 0.794985 1.248971 0.288416
H 2.326081 1.060866 -0.194422
O 3.778757 1.847775 -0.508441
H 4.126211 2.047101 -1.386809
H 4.533166 1.876521 0.093371

VIIa

-2314.292479
O -0.206430 0.007302 -1.594955
Zn -1.925405 -0.089646 -0.352493
O -1.183297 1.593237 0.776811
O -1.008759 -1.665159 0.810193
O 2.045791 1.559536 -1.059666
O 1.421906 1.349484 1.670433
O 1.689086 -1.393554 1.392667

O 2.574288 -1.184533 -1.151858
H -1.512364 -2.341484 1.279938
H -0.074311 -1.691830 1.116760
H 0.286375 -0.800186 -1.805161
H 0.472381 0.709940 -1.497882
H -0.318668 1.579959 1.246388
H -1.797607 2.137304 1.286193
H 1.801780 1.790252 2.441375
H 1.606683 0.388399 1.771889
H 2.167527 -1.987659 1.985339
H 2.129935 -1.457793 0.508339
H 2.344517 2.364769 -1.501036
H 1.983980 1.759189 -0.104049
H 3.273522 -1.660794 -1.616921
H 2.737746 -0.231181 -1.285381

VIIb

-2314.292152
O 1.855486 -0.545347 -0.153835
Zn 1.124889 1.291202 0.163769
O -0.856575 1.017126 -0.239008
O 4.421876 -1.190815 0.365590
O -2.202801 -1.319258 -0.821373
O 0.257077 -2.622506 -0.522756
O -2.573823 3.102175 -0.119055
H 1.312686 -1.365346 -0.308857
H 2.788997 -0.788115 0.047050
H -1.357517 0.190971 -0.433789
H -1.485056 1.775365 -0.190678
H -2.790495 3.570120 0.697328
H -2.656625 3.753582 -0.827125
H 4.805454 -1.416663 1.221802
H 5.161897 -1.093412 -0.246117
H -2.880247 -1.616054 -0.167772
H -2.648482 -1.322380 -1.678249
H -0.655471 -2.338602 -0.728415
H 0.450962 -3.389926 -1.073333
O -4.018334 -2.176629 1.001886
H -4.011767 -3.053077 1.406143
H -4.844260 -1.760497 1.277353

VIIc

-2314.291968
O -0.060513 1.728221 0.000223
O -0.166116 3.293594 -2.268056
O -1.411884 -0.606633 0.030971
Zn 0.069668 -1.988577 0.000554
O 1.450699 -0.506333 -0.029226
O -4.086438 -0.939878 0.016624
O 4.141839 -0.654864 -0.018825
H -0.064072 2.314942 0.786653
H -0.097878 2.313613 -0.786318
H 1.124045 0.424989 -0.019505
H 2.434507 -0.555314 -0.024850
H -2.389863 -0.724196 0.025115
H -1.151158 0.345235 0.020517
H -4.595337 -1.213800 -0.756633
H -4.600630 -1.215116 0.785910
H 4.669242 -0.892586 0.754011
H 4.672752 -0.894884 -0.788548
H -0.952159 3.717420 -2.633784
H 0.584881 3.699618 -2.717924
O -0.064214 3.299414 2.266962
H 0.690274 3.777683 2.632002
H -0.841639 3.651547 2.717345

VIId

-2314.289124
O -0.851228 1.041880 -0.269469
Zn 1.075556 1.376845 0.131749
O 1.817171 -0.524600 -0.061359
O -1.826222 -1.309468 0.265682
O -4.444248 -2.184239 0.410105
O -2.647304 3.073318 -0.291571
O 4.423564 -1.112169 0.286134
O 0.429645 -2.902242 -0.708253
H -1.303244 0.167189 -0.070556
H -1.508905 1.774158 -0.260174
H 1.341283 -1.348872 -0.292258
H 2.774435 -0.729008 0.065520
H 5.112994 -0.902066 -0.356494
H 4.858572 -1.125009 1.148135
H -2.896950 3.562534 -1.085250
H -2.895304 3.630837 0.456216
H 0.664798 -3.679225 -0.182456
H 0.470888 -3.195863 -1.628791
H -1.306385 -2.035743 -0.108947
H -2.761901 -1.596332 0.292747
H -5.161446 -2.059816 -0.223264
H -4.866544 -2.427966 1.242971

VIIe

-2314.288273
O -1.180993 1.235224 -0.023853
O 1.462984 0.580503 0.321867
Zn 1.534627 -1.303242 -0.480835
O -0.428541 -1.186092 -1.057253
O 3.456025 2.084981 1.318127
O -2.263556 -2.499710 0.377245
O -3.203045 -0.049871 1.687310

H -1.508470 2.026506 -0.507072
H -1.869623 0.996359 0.621782
H 0.601536 1.049780 0.346159
H 2.190084 1.135793 0.691108
H -1.078966 -1.811548 -0.647439
H -0.790861 -0.289309 -0.864263
H -2.847847 -3.243885 0.189691
H -2.788195 -1.832628 0.852109
H -3.065735 -0.061542 2.644889
H -4.114393 0.253444 1.571985
H 4.123553 2.525216 0.777164
H 3.858099 1.955375 2.186188
O -2.136745 3.415332 -1.372356
H -1.974809 4.340869 -1.151401
H -2.422212 3.409893 -2.294521

VIIf

-2314.287673
O 0.463498 1.660283 1.201975
O -1.869379 0.619967 -0.010839
Zn -1.435214 -1.392714 -0.122180
O 0.320496 -1.125359 0.850691
O 2.566263 -2.102402 -0.010206
O 3.972604 0.075540 -0.898826
O 2.777223 2.707083 -0.123288
H 0.406758 2.049098 2.084512
H 1.227694 2.090711 0.767105
H -1.210625 1.242923 0.349578
H -2.712622 1.085812 -0.230373
H 1.179765 -1.562763 0.563336
H 0.521090 -0.197519 1.088005
H 3.121873 -2.721123 0.478024
H 3.151854 -1.390026 -0.348603
H 2.605276 3.350551 -0.825255
H 3.437557 3.128987 0.444935
H 3.628316 0.975402 -0.781590
H 4.561706 0.099476 -1.662040
O -4.160713 1.879291 -0.600539
H -4.944719 1.866770 -0.037118
H -4.477440 2.047898 -1.496853

VIIIa

-2390.731489
O 1.470763 0.886023 -1.092227
Zn 2.087858 -0.896830 -0.119261
O 1.518192 -0.047880 1.786958
O 0.234417 -1.834151 -0.645255
O -2.028275 -0.478670 -0.042626
O -0.913183 1.239688 1.907070
O -0.342035 3.107985 0.030806
O -1.139412 1.307182 -1.930122
H 1.916178 -0.331193 2.619298
H 0.656491 0.390327 1.979725
H 1.565415 1.730416 -0.626536
H 0.605569 0.940471 -1.556026
H -0.651690 -1.473525 -0.387642
H 0.176744 -2.796876 -0.682347
H -2.919448 -0.881583 0.059009
H -1.851551 0.045851 0.763901
H -1.320511 1.539766 2.729441
H -0.761961 2.046150 1.354776
H -1.485290 1.312902 -2.831013
H -1.650998 0.638399 -1.420724
H -0.430338 4.068927 0.043784
H -0.787941 2.788236 -0.777804
O -4.505804 -1.603928 0.216610
H -4.721755 -2.458456 0.609750
H -5.331948 -1.264911 -0.149465

VIIIb

-2390.731173
O -4.663878 0.683658 -0.585208
Zn -0.990004 -1.181526 0.397500
O 0.404356 -0.334594 1.849919
O -2.032850 0.601876 0.049192
O 0.367374 -0.742852 -1.191477
O 3.086039 -1.701046 -1.036464
O 1.661270 1.996928 1.017074
H 1.281461 -1.084091 -1.176663
H 0.398315 0.207775 -1.429103
H -1.565663 1.270459 -0.487814
H -2.989773 0.612887 -0.187204
H -5.126515 0.059546 -1.158156
H -5.334086 1.051880 0.003960
H 0.812598 0.547393 1.687555
H 0.176682 -0.383787 2.787287
H 3.447598 -2.010215 -1.879086
H 3.174181 -2.452443 -0.433118
H 2.544158 1.672597 0.704403
H 1.832876 2.738389 1.611109
O 3.856646 0.896570 -0.053199
H 4.797302 1.068171 0.069864
H 3.770364 -0.021908 -0.365109
O 0.039182 2.001994 -1.214810
H 0.630862 2.252105 -0.472018
H 0.104633 2.696732 -1.881137

VIIIc

-2390.730894
O 0.843819 -1.123138 -1.557554
Zn 2.141010 -0.235868 -0.085541

O 0.829580 -0.669046 1.522556
O 1.419592 1.784396 -0.141900
O -1.820036 -1.735188 -1.180621
O -1.356696 0.882193 2.166683
O -1.263311 2.396276 -0.125331
H 1.979713 2.458536 -0.547116
H 0.479019 2.066316 -0.243643
H 1.212396 -1.537409 -2.347665
H -0.094809 -1.412134 -1.463971
H 0.153348 -0.030233 1.844327
H 0.440614 -1.547451 1.639821
H -1.467753 1.356616 3.000276
H -1.441625 1.546625 1.444508
H -1.523173 3.324908 -0.178277
H -1.788665 1.916886 -0.823197
H -2.191251 -2.518078 -1.607385
H -2.000621 -1.832879 -0.212345
O -2.515567 0.894755 -1.913708
H -3.348068 1.036540 -2.378467
H -2.421767 -0.066928 -1.766410
O -2.065709 -1.752907 1.518198
H -2.700677 -2.264848 2.034276
H -2.090353 -0.839148 1.864917

VIIId

-2390.729156
O 4.139035 1.099593 -0.743601
O 1.625696 0.681949 0.224335
Zn 0.105362 -0.012676 -1.097694
O -1.483347 0.863048 0.028341
O 0.079444 -1.855159 -0.077057
O -2.917637 2.923680 -1.050109
O 0.899853 -0.904309 2.442005
O -1.035278 1.119743 2.930312
H -0.538220 -2.595507 -0.271075
H 0.244463 -1.817069 0.882949
H 1.715410 0.135654 1.027735
H 2.527703 0.838504 -0.137997
H 4.518024 0.611473 -1.485247
H 4.596321 1.949413 -0.724216
H -1.346757 1.078871 0.968002
H -1.988957 1.604067 -0.376843
H -2.533771 3.560695 -1.665994
H -3.834250 2.808562 -1.331156
H -1.846359 0.965643 3.434350
H -0.693302 1.965072 3.253195
H 0.250939 -0.290300 2.835592
H 1.351815 -1.341535 3.173948
O -1.550153 -3.975723 -0.599761
H -2.465749 -3.936513 -0.902622
H -1.179074 -4.779322 -0.985506

VIIIe

-2390.727090
O 1.737380 -0.489311 -0.119803
Zn 0.455378 -2.011221 -0.190800
O -1.336050 -1.072068 0.079552
O 1.009409 1.893970 0.583437
O 4.415779 -0.924481 0.081892
O -3.656143 -2.477562 -0.012348
O -1.802494 1.499002 0.895584
H 1.501649 0.458207 0.131201
H 2.705416 -0.635096 -0.032426
H -1.523620 -0.147292 0.370108
H -2.178252 -1.581922 0.053880
H -4.013872 -2.823326 -0.839957
H -3.921331 -3.105478 0.671690
H 4.996624 -1.151546 -0.654520
H 4.904196 -1.138575 0.886163
H -2.057243 1.602920 1.821277
H -2.453036 2.029328 0.380589
H 0.043179 1.979490 0.657912
H 1.355141 2.729875 0.212043
O 1.967946 4.325463 -0.382787
H 2.341391 4.484972 -1.258377
H 2.447241 4.912849 0.215004
O -3.570103 2.996122 -0.545167
H -4.489160 2.789157 -0.754021
H -3.445469 3.923994 -0.779451

VIIIf

-2390.725452
O 0.457442 1.570655 0.218572
O -1.875235 0.285661 -0.437348
Zn -1.537102 -1.608766 0.279524
O 0.247438 -1.047541 1.051447
O 2.429954 -2.398991 0.585462
O 3.892174 -0.826974 -1.115912
O 2.741870 1.855351 -1.580812
H 0.491992 2.295929 0.880466
H 1.186292 1.737083 -0.406730
H -1.170946 0.960255 -0.325923
H -2.696345 0.676466 -0.817068
H 1.077406 -1.599957 0.938931
H 0.476977 -0.111255 0.855375
H 2.984868 -2.797999 1.265530
H 3.025985 -1.905055 -0.020022
H 2.538478 2.112823 -2.490730
H 3.389412 2.506638 -1.276182
H 3.550545 0.040382 -1.390302
H 4.450036 -1.146047 -1.834808
O -4.130523 1.338939 -1.479329

H -4.925788 1.518746 -0.962242
H -4.433187 1.162519 -2.379006
O 0.629274 3.591779 2.072101
H 0.913359 3.452879 2.984325
H 0.114838 4.408532 2.079212

VIIIg

-2390.725422
O 1.125152 -0.281376 0.139147
O -0.903395 1.485179 0.325414
Zn -2.523177 0.288007 0.071586
O -1.340693 -1.361404 0.151529
O -1.996322 -3.928823 -0.347117
O -0.732905 4.129117 -0.169355
O 3.367644 -0.581929 2.017683
O 2.721766 -0.072382 -1.975150
H 1.664652 -0.252754 -0.698749
H 1.776446 -0.405104 0.852459
H -0.023370 1.040475 0.261551
H -0.833633 2.448031 0.126838
H -1.573650 -2.298036 -0.046411
H -0.364952 -1.212868 0.128242
H -2.354809 -4.521803 0.325021
H -2.279161 -4.286812 -1.197769
H -0.717418 4.552447 -1.036576
H -0.986656 4.814769 0.460784
H 3.525507 -1.462664 2.384752
H 3.413733 0.017035 2.775314
H 3.621681 -0.078636 -1.580129
H 2.756937 -0.651856 -2.744832
O 4.960050 -0.188147 -0.421525
H 4.653216 -0.217886 0.499378
H 5.806404 0.273560 -0.422466

VIIIh

-2390.720275
O -1.952599 2.963910 -0.544239
Zn -0.687308 -0.517037 -0.306792
O -0.107413 -0.987037 1.665925
O 2.579251 -1.124348 -2.065858
O -2.475046 0.494307 0.193682
O 0.461767 1.627203 0.124223
O 3.093071 0.885786 -0.343462
H 1.398408 1.514287 -0.156392
H 0.523783 1.812933 1.073373
H -2.693648 0.538750 1.135338
H -2.447951 1.436549 -0.129059
H -0.985657 2.909828 -0.618733
H -2.267866 3.600189 -1.196724
H 2.983036 -1.439675 -2.884416
H 1.618858 -1.185495 -2.190096
H 0.812613 -0.716186 1.932921
H -0.255512 -1.893611 1.964952
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H 3.057854 0.181097 -1.034599
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H -3.015093 -2.098873 -0.287870
H -1.941320 -3.131707 -0.694418
H 2.808146 0.254632 1.383735
O 2.279997 0.046475 2.181519
H 2.898056 -0.152905 2.894392

Xa

-2543.606781
O 0.967294 -1.811602 -2.038188
O -0.620650 0.423826 -1.568392
Zn -2.287456 0.389730 -0.289947
O -1.686721 -1.372922 0.767622
O -1.411192 1.613742 1.284438
O 1.355270 2.372817 -1.568753
O 1.197214 2.562023 1.223304
O 2.627129 0.240017 1.527802
O 2.940740 0.000388 -1.059104
O 0.747070 -1.700889 2.125908
O 0.304450 -3.489105 0.018012
H -0.889070 -1.334410 1.338713
H -1.632453 -2.232781 0.322915
H -2.007085 2.193359 1.775997
H -0.518012 2.029174 1.287734
H 1.462660 3.301025 1.785618
H 1.775473 1.799137 1.470747
H -0.007975 1.183414 -1.668697
H -0.121327 -0.391835 -1.793402
H 3.483941 0.205584 1.972757
H 2.815491 0.098406 0.548168
H 1.352488 2.710830 -0.650266
H 1.439902 3.135563 -2.154463
H 2.413358 -0.708330 -1.474957
H 2.614401 0.827520 -1.454830
H 0.771460 -2.528346 -1.389899
H 1.006237 -2.228827 -2.908028
H 0.648494 -3.091054 0.842555
H 0.471845 -4.438050 0.072785
H 1.456327 -1.026658 2.003887
H 0.722697 -1.901996 3.069890

Xb

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O 0.127002 1.661903 1.504179
O -1.889622 1.333297 -0.717569
O -2.097706 -1.287720 -0.135712
O -0.010337 -2.590222 -1.209350
O -1.234742 -0.593768 2.330174
O 2.193278 -1.214247 -0.212442
O 1.553146 -0.774132 2.442639
O -4.554814 -2.447988 -0.645578
H -2.525992 1.633564 -1.377646
H -1.998905 0.351279 -0.603398
H 1.807677 1.321051 -2.104199
H 1.707090 0.256782 -0.925943
H -0.515438 0.992880 1.832213
H 0.988307 1.346136 1.819078
H -1.896611 -0.634579 3.030932
H -1.657374 -0.954250 1.509803
H -2.957071 -1.723766 -0.316687
H -1.394926 -1.845293 -0.556957
H 3.118972 -1.486353 -0.388571
H 2.092414 -1.154060 0.762686
H 0.104220 -3.540059 -1.323667
H 0.847740 -2.233205 -0.896112
H 2.018978 -1.099441 3.222346
H 0.601544 -0.948741 2.588932
H -4.985111 -2.499627 -1.507863
H -5.080022 -3.003512 -0.056772
O 4.793905 -1.963360 -0.754149
H 5.580797 -1.406008 -0.717215
H 5.098801 -2.830663 -1.047331

Xc

-2543.605844
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O -3.960703 -0.188348 -2.645022
O 2.451757 -0.343986 0.260264
O -0.296754 -1.494511 -0.253298
O -3.099513 -1.465121 -0.396522
O -0.794565 0.822495 2.605539
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H -0.056802 -1.683670 0.676638
H 2.137814 -0.775067 1.079327
H 3.262457 -0.814174 -0.037825
H 4.765349 -2.247976 -1.291394
H 5.602990 -1.309586 -0.401519
H -4.847631 0.129307 -2.853759
H -3.464100 -0.160038 -3.472125
H -0.258908 1.420093 0.939846
H 0.336882 2.497288 -0.060022
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H -3.430986 -1.004040 -1.201812
H 1.866895 4.384275 -0.174845
H 0.464875 4.857099 -0.600582
H -1.733679 0.517386 2.505469
H -0.787407 1.467060 3.323529
O -3.201527 -0.229518 2.118839
H -4.079602 0.015375 2.430859
H -3.309706 -0.620617 1.228145
O 0.805112 -1.375021 2.297054
H 0.282032 -0.616697 2.642117
H 0.930230 -1.992573 3.027273

Xd

-2543.605543
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O 0.923327 -1.056975 -1.285355
O -2.053246 1.368415 -0.135188
O -1.002894 1.901586 2.292669
O 0.096214 1.530273 -1.803445
O 1.503815 0.601096 2.215597
O 2.456415 1.078746 -0.242493
H -2.866004 -1.700379 -0.487831
H -2.093374 -0.320424 -0.359510
H 0.408110 -2.459167 2.400556
H 0.758084 -0.980607 1.962570
H 0.481227 -0.276879 -1.685929
H 1.713883 -0.667401 -0.866344
H -0.050290 1.975414 -2.646548
H -0.736028 1.627152 -1.280293
H -2.908337 1.822478 -0.289705
H -1.746620 1.632816 0.766929
H 2.162051 0.685317 2.916543
H 1.956341 0.855394 1.368669
H -1.058410 2.708385 2.816736
H -0.096066 1.553848 2.399540
H 3.350598 1.418050 -0.463010
H 1.814111 1.560306 -0.795353
O 5.001529 1.934806 -0.816820
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H 5.422026 2.778928 -0.612666
O -4.491281 2.588483 -0.605526
H -5.311532 2.409793 -0.129435
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Xe

-2543.605483
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O 0.939773 -2.361919 0.031346
O 0.532189 1.420939 1.077779
O 2.107100 -0.041236 -0.679798
O 4.848736 0.079734 -1.008504
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H -0.440687 0.187581 1.725572
H -1.151357 -0.687255 2.846988
H 0.927282 2.109100 1.652561
H 1.257586 1.019515 0.551018
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H 1.678088 0.177122 -1.538202
H -2.082901 2.258240 -1.007397
H -0.787159 1.814390 -0.208254
H 0.572657 0.787515 -3.675789
H -0.219730 1.119349 -2.366968
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O -3.450485 3.388120 -1.024123
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O 1.623858 3.382970 2.693748
H 1.953832 3.274538 3.594086
H 1.475999 4.329955 2.581057

Xf

-2543.604362
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Zn 0.000021 -1.582300 -0.148131
O -0.000074 -0.569069 1.700910
O 2.526942 -1.276741 -0.098266
O -2.527059 -1.276693 -0.098462
O -2.532110 0.517189 1.948421
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H 2.722594 -0.785231 0.733933
H 0.799291 -0.044076 1.918215
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H 3.022836 0.572956 2.777041
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H -2.954987 -2.140171 -0.025889
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H -2.845146 -0.082243 -1.496935
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H -3.418568 3.306502 0.198343

Xg

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H 2.999004 -0.170890 -2.475387
O -3.097507 0.078874 -0.445462
H -3.972173 -0.329208 -0.484180
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H 3.938724 -1.779965 0.984129
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H -2.578278 2.906967 1.661452
H -1.670475 2.605591 0.417538
O -0.354866 -0.175196 -1.548679
H -0.562123 0.776844 -1.511426
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H 0.433045 2.807920 -0.815652
H -0.718284 3.326460 -1.732234

References

1. N.K. Bersenkowitsch, M. Ončák, J. Heller, C. van der Linde and M.K. Beyer, *Chem. Eur. J.*, 2018, **24**(47), 12433.
2. J. Heller, M. Ončák, N.K. Bersenkowitsch, C. van der Linde and M.K. Beyer, *Eur. J. Mass Spectrom.*, 2019, **25**, 122-132.