Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Size-Dependent H and H_2 Formation by Infrared Multiple Photon Dissociation Spectroscopy of Hydrated Vanadium Cations, $V^+(H_2O)_n$, n = 3–51

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IRMPD Spectra of Small Clusters

The measured IRMPD spectra below, along with the simulated structures and spectra, are consistent with findings from Ohashi and Duncan.[1,2] A direct comparison between IRMPD spectra of the present study with those measured by Duncan can be found in Figure 1 of the main article.

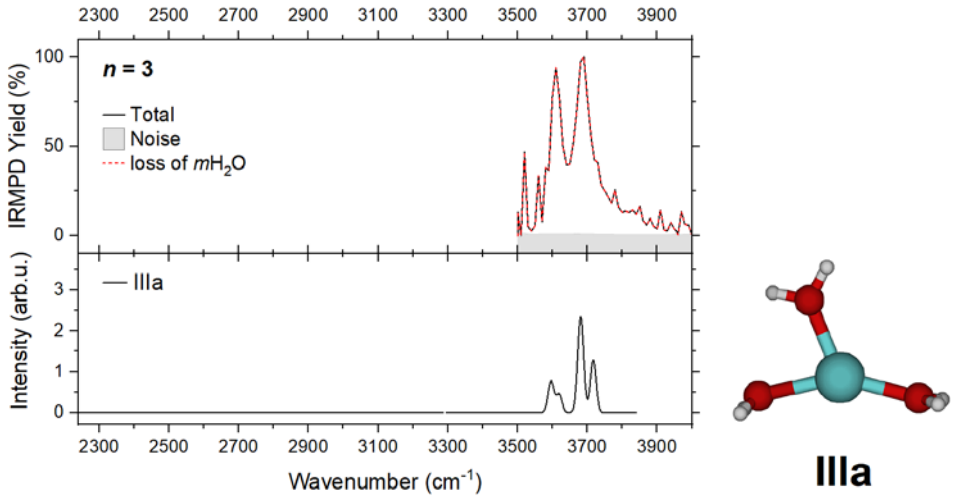

Figure S1. Infrared multiple photon dissociation spectrum of the $V^+(H_2O)_3$ complex along with the simulated spectra of the low-lying intact (**IIIa**) isomer calculated at the B3LYP/aug-cc-pVDZ level of theory.

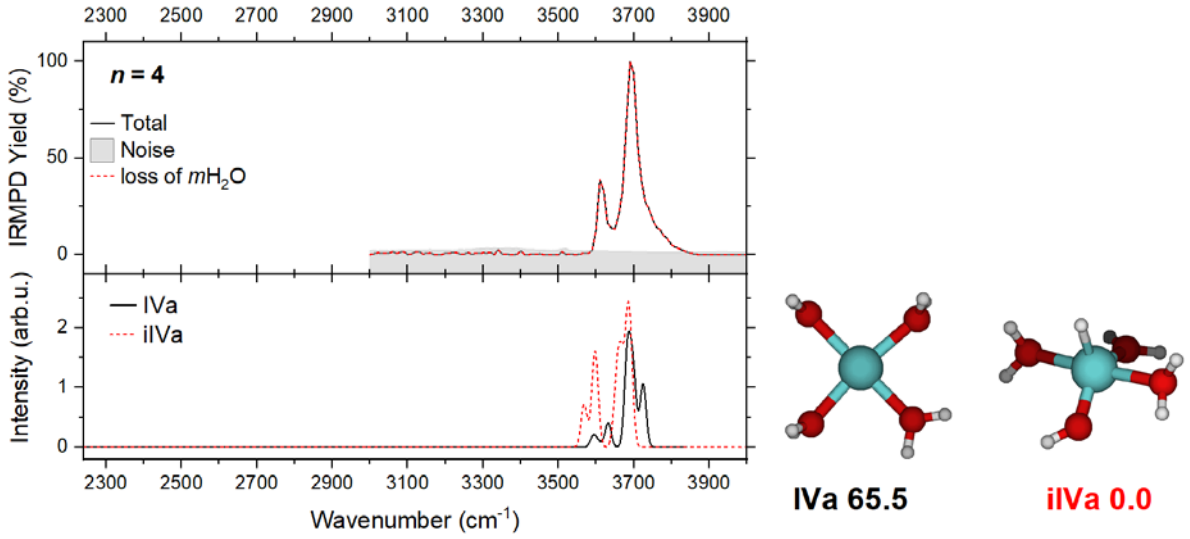

Figure S2. Infrared multiple photon dissociation spectrum of the $V^+(H_2O)_4$ complex along with the simulated spectra of the low-lying intact (**IVa**) and inserted (**iIVa**) isomers calculated at the B3LYP/aug-cc-pVDZ level of theory. Structural isomers also show relative energies given in kJ mol^{-1} inclusive of zero-point energy.

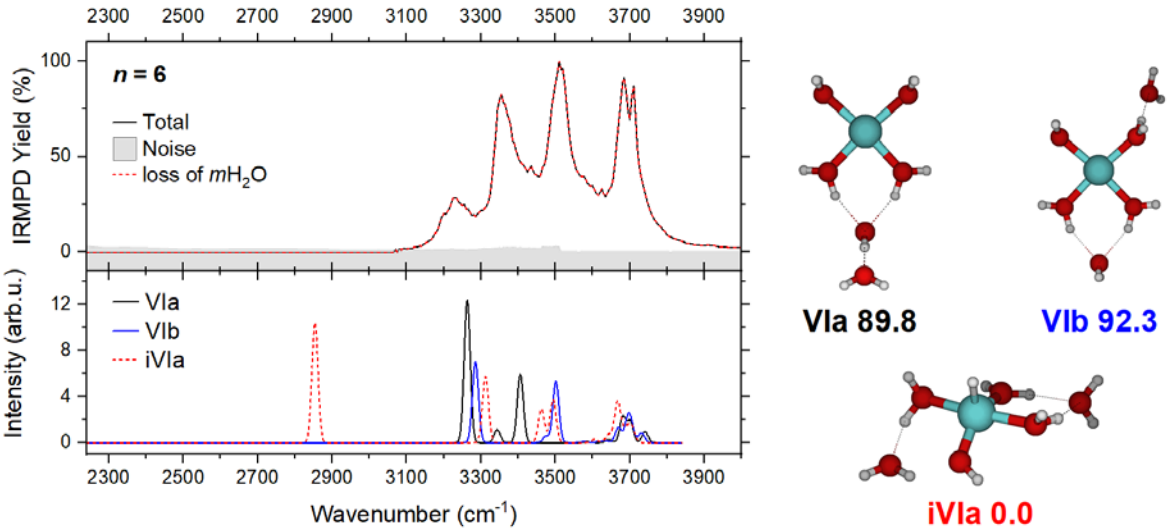

Figure S3. Infrared multiple photon dissociation spectrum of the $V^+(H_2O)_6$ complex along with the simulated spectra of the low-lying intact (**VIa, VIb**) and inserted (**iVIa**) isomers calculated at the B3LYP/aug-cc-pVDZ level of theory. Structural isomers also show relative energies given in kJ mol^{-1} inclusive of zero-point energy.

Ligand Fragmentation

Table S1 – Number of ligands lost during the IRMPD process for each cluster size, $V^+(H_2O)_n$ (n = 3–12, 14, 15, 20, 25, 30, 42 and 51), consistent with measured black body infrared dissociation (BIRD) values.[3]

$V^+(H_2O)_n$	$m(H_2O)$	H + $x(H_2O)$	H_2 + $y(H_2O)$
3	1	–	–
4	1	–	–
5	1	–	–
6	1,2	–	–
7	1,2	–	–
8	1,2	–	1
9	1,2	0,1	1,2
10	1,2	0,1	2
11	1,2	0,1	1,2
12	1	–	2,3
14	1	–	2,3,4
15	1,2,3	–	3
20	1,2,3,4	–	–
25	1,2,3,4	–	–
30	1,2,3,4,5	–	–
42	1,2,3	–	–
51	1,2,3	–	–

References

1 J. Sasaki, K. Ohashi, K. Inoue, T. Imamura, K. Judai, N. Nishi and H. Sekiya, *Chem. Phys. Lett.*, 2009, **474**, 36.

2 P. D. Carnegie, J. H. Marks, A. D. Brathwaite, T. B. Ward and M. A. Duncan, *J. Phys. Chem. A*, 2020, **124**, 1093.

3 B. S. Fox, I. Balteanu, O. P. Balaj, H. C. Liu, M. K. Beyer and V. E. Bondybey, *Phys. Chem. Chem. Phys.*, 2002, **4**, 2224.

Cartesian structures of optimized ions (Å) along with ZPE-corrected energies (Hartree)

```
IIIa
E = -1173.103678
O 2.330794 -0.132725 -0.000142
V 0.213123 -0.142249 0.000179
O -1.058361 1.591990 -0.000542
O -1.739995 -1.130670 0.000002
H -2.062824 -1.611282 -0.775974
H -2.061265 -1.615427 0.774030
H 2.903368 -0.096855 -0.780030
H 2.903689 -0.096167 0.779475
H -2.023711 1.535106 0.002890
H -0.820593 2.527587 0.000955

IVa
E = -1249.557986
O -0.521866 -2.071034 0.000138
V 0.004612 0.029990 -0.000030
O -2.159259 0.417555 -0.000289
O 0.569618 2.148692 0.000194
O 2.091808 -0.657801 0.000130
H 0.098495 -2.810769 0.002927
H -1.414797 -2.437914 -0.001204
H 2.662546 -0.544535 0.773527
H -2.625454 0.759361 0.775737
H 2.659965 -0.551879 -0.776211
H -2.624621 0.762328 -0.775499
H 0.645717 2.717683 0.777783
H 0.649667 2.716649 -0.777759

iIVa
E = -1249.582933
O -2.114704 -0.203523 0.193675
V -0.012727 0.103277 0.211674
O 0.246513 -1.841736 -0.462338
O -0.356143 1.637637 -0.658842
O 2.131221 0.199309 0.196030
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H -2.519960 0.561016 -0.249296
H 0.257915 2.338005 -0.917522
H -0.462381 -2.439138 -0.742144
H 2.511194 0.401631 1.064365
H 2.654864 0.685668 -0.457349
H 0.086844 0.347917 1.848531
H 1.095281 -2.288119 -0.595873

Va
E = -1326.000340
O 2.041927 -1.655097 0.014051
V 0.597029 0.000103 0.000988
O -0.986991 -1.473599 -0.049081
O 2.042016 1.655169 0.013784
O -0.987281 1.473579 -0.047125
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H -1.928787 -1.230014 0.007023
H 2.554802 1.911434 -0.765685
H -0.904265 -2.427076 0.066670
H 2.572904 1.886046 0.788860
H -1.929803 1.232008 0.004805
H -0.904174 2.428879 0.051789
O -3.402052 -0.000225 0.035025
H -3.991535 -0.001638 -0.732394
H -3.987505 0.000406 0.805363

Vb
E = -1325.997426
O 3.679063 -0.141104 -0.608385
V -0.602970 0.027119 0.137021
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O -0.891302 2.181174 -0.122546
O -0.269479 -2.134473 0.227668
O -2.631020 -0.471648 -0.567220
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H -0.937443 -2.730489 -0.138327
H -2.951829 -0.170668 -1.429393
H -3.393903 -0.469867 0.028664
H 2.236982 0.248782 0.216892
H 1.685165 0.604141 1.641692

Vc
E = -1325.988819
O 1.903491 -0.021790 -0.266750
H 2.602523 0.590917 -0.525972
H 2.298538 -0.921798 -0.179162
V -0.051691 0.662188 0.202049
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H 1.029008 3.257453 0.306776
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H -2.047778 -0.359470 1.773698
O 2.929349 -2.488822 -0.018927
H 3.456766 -2.797823 0.728331
H 3.138644 -3.075273 -0.756692
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H -3.893773 -2.175299 -0.860498
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iVa
E = -1326.030297
O 0.495591 -1.884174 0.384740
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O -1.765206 1.733748 0.074854
O 0.975251 1.044336 -0.032199
O -1.665100 -1.088987 -0.921599
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H 0.023312 -2.556215 -0.134890
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H -2.490577 -0.845600 -1.360088
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H 3.911121 0.087698 -1.088053
H 4.178048 0.559045 0.364239
H -1.257398 -0.194418 1.785997
H -2.315294 1.973173 -0.684717

iVb
E = -1326.028389
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O -3.004182 -0.308127 -0.527930
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VIa
E = -1402.439937
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O 2.665848 1.651059 -0.259498
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H 3.353125 1.858752 0.388684
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H -5.216105 -0.772039 -1.122135

VIb
E = -1402.438963
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O -1.042011 -1.581518 0.182914
O 0.865104 2.340090 0.074250
O -3.766093 -0.932472 -0.275448
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H 1.480678 2.561099 -0.639677
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H -0.990466 -2.480180 -1.198082
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VIIId
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iVIIIa
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H -3.520854 2.088879 0.668768

iVIIIb
E = -1555.357661
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O -2.853735 -1.302094 -0.532571
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H 1.198245 -1.733229 1.765886

iVIIIc
E = -1555.357067
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O -2.365838 -0.317608 -1.040191
O -0.110282 -1.813249 -0.297443
O -0.292881 1.698718 -0.502022

O 2.393380 -2.030880 0.360131
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H 2.565887 3.033830 0.468277
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H -4.513810 0.286643 1.159197
H 4.317272 0.042014 -1.523962
H 2.940689 -2.775214 0.638128
H 2.956616 -1.416032 -0.182548
H -1.839452 0.205206 1.441455

iVIIId
E = -1555.353271
O 1.000912 -1.881451 -0.564151
V -0.674119 -0.703756 0.020327
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O -0.784227 -1.790373 1.459235
O 2.949525 0.066852 -1.017496
O 5.138373 0.374359 0.532248
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H 1.109399 -2.643773 0.022189
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H 0.229044 1.859457 -0.176197
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H 3.762883 0.189301 -0.469122
H -1.690606 -1.276430 -1.184473

IXa
E = -1631.753600
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V -0.045427 -0.343544 -0.299676
O 1.483359 1.127156 0.166035
O 1.506016 -1.887951 -0.227795
O -1.520382 1.231601 -0.480147
O -3.932176 -0.173734 -0.514229
O -5.630762 -0.665728 1.570943
O 3.803468 -0.314434 -0.474304
O 0.017628 3.622818 0.023190
H -2.543603 -1.379974 -0.686186
H -1.578282 -2.362040 -1.432041
H 2.410902 -1.510562 -0.266054
H -2.470436 1.032132 -0.388406
H 1.487520 -2.499457 0.520827
H -1.331385 2.143073 -0.208030
H 2.406443 0.920397 -0.072389
H 1.304062 2.070304 0.024046
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H 4.151078 -0.293437 -1.375104
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H -4.512457 -0.054124 -1.276709
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H -6.074755 -0.032735 2.148057
O 5.988555 -0.542422 1.162668
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H 6.514081 -1.338000 1.311463

IXb
E = -1631.753268
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V 0.318923 -1.001096 -0.001629
O 2.099477 0.234454 0.175623
O 1.450003 -2.738455 0.718882
O -0.727376 0.713658 -0.781237
O -3.396205 -0.149940 -0.855503
O -5.425003 0.344155 0.914595
O 4.086327 -1.904631 -0.006903
O 1.247095 2.706350 -0.830512
H -2.319794 -1.570678 -0.415339
H -1.580842 -2.939128 -0.611861
H 2.414767 -2.629730 0.611711
H -1.698339 0.765711 -0.815559
H 1.298205 -3.010205 1.635022
H -0.318169 1.596836 -0.802684
H 2.960170 -0.163324 -0.028078
H 2.049384 1.128412 -0.217446
H 4.882448 -1.961529 0.539405
H 4.342146 -2.267166 -0.866662
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H 1.327511 3.493537 -0.247388
H 1.499044 3.013682 -1.710403
H -5.839621 -0.322299 1.475992
H -5.798874 1.191460 1.184936
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H 2.234626 5.089813 1.384953

IXc
E = -1631.752627
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O 0.721328 1.832809 0.132003
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O -2.137720 -1.356239 -0.767339
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H 1.837912 -0.562010 -0.895427
H 1.111734 -1.847407 -0.381001
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H 3.834905 0.581865 -0.127045
H 3.486020 1.020067 -1.588749
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H -5.237587 -0.404330 0.242753
H -5.090459 0.237877 -1.165502
O 5.036551 0.304980 0.971549
H 5.816814 -0.274577 0.844041
H 5.258837 0.915686 1.682787
O -6.392366 -1.007092 1.391364
H -6.626218 -1.933360 1.528003
H -7.011980 -0.492843 1.923216
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IXd
E = -1631.749201
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O 3.277371 -1.792734 -0.080481
O 3.912919 1.241259 0.005085
O 0.248530 -1.133279 -0.224819
O -1.572892 0.835078 -0.775665

O -3.638909 1.126521 0.807718
O -5.597252 -0.707322 0.919434
O 5.910833 -0.772285 0.385160
H 4.041601 1.951001 -0.638407
H 4.756227 0.756829 0.073785
H 4.243316 -1.690817 0.004097
H 3.118023 -2.458109 -0.763308
H 0.012271 -1.720698 0.505029
H -0.546046 -0.583585 -0.418938
H -0.067801 1.693700 -0.345677
H 0.900099 2.458021 0.624277
H -2.382968 0.960767 -0.200258
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H 6.224217 -0.863397 1.296240
H 6.690945 -0.919387 -0.167560
H -4.007113 1.981603 1.054834
H -4.381852 0.475308 0.850486
H -5.823113 -1.152614 1.743537
H -6.408848 -0.713256 0.372468
O -7.864074 -0.717905 -0.686064
H -8.114432 -1.449640 -1.263097
H -8.664631 -0.193553 -0.562666

IXe
E = -1631.748298
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O 3.361048 -1.551263 -0.100653
O 0.295099 1.531861 0.356843
O 3.361081 1.551300 -0.100806
O -1.807968 -0.000043 1.167491
O -4.019711 0.000005 -0.188820
O -5.528597 -2.348222 -0.485667
O 5.685906 -0.000087 -0.721258
H 3.399127 -2.257540 0.558246
H 4.275610 -1.251371 -0.255977
H 4.275580 1.251256 -0.256186
H 3.399297 2.257528 0.558134
H 0.107046 2.131368 -0.377083
H -0.569427 1.157907 0.650767
H -0.569413 -1.157839 0.650918
H 0.107022 -2.131518 -0.376800
H -2.683639 -0.000046 0.669764
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H 5.936009 -0.000105 -1.656129
H 6.521953 -0.000020 -0.234706
H -4.586746 -0.787703 -0.288418
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H -6.165245 -2.706539 0.144812
H -5.780865 -2.710036 -1.343992
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iIXa
E = -1631.798859
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O 2.263699 -0.066879 -0.751170
O -2.714832 -1.986056 -0.583139
O -3.636588 0.635706 -0.930830
O 4.254356 -1.296733 0.499982
O -2.355153 1.835400 1.052824
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H -1.952992 -1.330317 0.917261
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H 0.749142 2.174716 0.005288
H -1.799126 -2.052657 -0.956725
H -0.727695 1.856428 0.645174
H 0.471226 -1.845147 -1.734269
H 2.497983 0.858203 -0.932255
H 3.066403 -0.518330 -0.378291
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H 2.814973 3.396524 -0.392912
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H -2.953074 1.530278 0.318967
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iIXb
E = -1631.798034
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V -0.672343 0.423439 -0.155837
O -2.337211 -0.681729 -0.971787
O 1.030346 1.372981 0.620877
O -1.806223 1.237115 1.041472
O 2.740414 -0.815481 1.103817
O 5.038087 -1.199662 -0.268396
O 1.694463 3.416402 -0.964178
O -1.220009 -3.357827 -0.388542
O -4.251502 0.296221 0.445964
H 1.238050 -1.355016 0.402383
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H -3.179055 -0.434839 -0.466707
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iIXc
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iIXd
E = -1631.796120
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V 0.715860 -0.468968 0.149438
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O -4.631641 1.428073 -1.524499
O -0.875341 -3.690637 1.268134
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H 4.679846 -0.178154 -1.618269
H -3.639594 0.821488 -0.264437
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H -0.902986 -4.639126 1.090845
H -0.002526 -3.504263 1.645794
H -5.092903 2.275555 -1.549282
H -5.040910 0.881087 -2.206650
H 1.181006 3.589262 2.223085
H 1.148950 4.078104 0.764784
H 1.056084 -1.614499 1.319130

H2O
E = -76.423418
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H -0.000000 0.764237 -0.471206
H -0.000000 -0.764237 -0.471206

H
E =
H 0.000000 0.000000 0.000000

H2
E = -1.164102
H 0.000000 -0.000000 0.380433
H 0.000000 -0.000000 -0.380433

V+(H2O)7
E = -1478.878329
O -2.123928 -1.556000 0.320856
V -0.620010 -0.000051 -0.034483
O -2.123656 1.556188 0.321324
O 0.901576 1.517798 -0.396507
O 0.901986 -1.517082 -0.396797
O 3.175027 0.000085 -0.859025
O 5.152405 -0.000516 0.994611
H -2.027442 -2.136033 1.088752
H -3.051378 -1.253416 0.306363
H 1.796102 -1.181238 -0.621527
H -2.026309 2.138025 1.087737
H 0.721614 -2.270710 -0.972879
H -3.051199 1.253912 0.308404
H 1.795740 1.181754 -0.620651
H 0.721436 2.270781 -0.973514
H 3.887124 -0.000125 -0.175809
H 3.633825 0.000581 -1.708842
H 5.555550 0.771244 1.410657
H 5.555019 -0.772284 1.411156
O -4.517574 -0.000431 0.066291
H -5.274321 -0.002108 0.669186
H -4.902221 0.000447 -0.821949

HVOH+(H2O)6
E = -1478.917497
V -0.151336 -0.892274 -0.380030
H -0.450864 -2.168297 -1.412129
O 0.706536 -1.329401 1.186140
H 0.202288 -1.647546 1.947614
O 1.690143 -0.527212 -1.337583
H 2.005462 -1.212988 -1.940826
H 2.414912 -0.303624 -0.707363
O 2.860982 0.278958 0.923261
H 3.704943 0.189818 1.382859
H 2.225862 -0.352981 1.337319
O 1.316386 2.522944 0.087335
H 2.008308 1.944615 0.465064
H 1.763424 3.247942 -0.365926
O -0.669756 1.040727 -0.668393
H 0.063657 1.710637 -0.493784
H -1.521426 1.391854 -0.344594
O -3.307929 1.321854 0.315701
H -4.008282 1.559615 -0.308775
H -3.530571 1.785834 1.135484
O -2.106491 -1.202707 0.427430
H -2.565975 -1.997522 0.125557
H -2.749987 -0.466348 0.449051

VOH+(H2O)4
E = -1325.454518
O 1.996174 0.884367 -0.050629
V 0.099944 -0.180795 -0.065913
O -0.633408 1.233297 1.457863
O -1.123811 1.181730 -1.318768
O 1.366308 -1.571134 -0.077907
O -1.697660 -1.379443 0.177755
H 2.394525 1.475141 -0.702235
H 2.498868 0.041644 -0.066126
H -1.448632 2.022260 -0.966108
H -1.072533 1.278352 -2.278540
H 1.375266 -2.529400 0.000301
H -1.598119 -2.322235 0.369384
H -2.468377 -1.295673 -0.400160
H 0.045605 1.733201 1.933578
H -1.286141 0.964447 2.119406

VOH+(H2O)5
E = -1401.904594
O 1.359888 1.417852 -0.935355
V 0.020338 -0.019943 0.027738
O 1.708073 -0.227950 1.453787
O -1.688039 0.130658 -1.043249
O 0.933698 -1.634251 -1.124540
O -0.975961 1.818499 0.681867
O -1.388483 -1.464655 0.875944
H 1.734170 1.265550 -1.813668
H 1.011335 2.321344 -0.933511
H 0.323709 -2.167742 -1.653082
H -1.679159 1.553029 0.028421
H 1.566200 -2.251841 -0.733040
H -1.395678 2.097168 1.504693
H -1.854695 -1.517740 1.718834
H -2.023886 -1.148621 0.182515
H -1.859014 0.170516 -1.988273
H 1.685753 -0.599047 2.344856
H 2.430082 0.414849 1.436638

VOH+(H2O)6
E = -1478.352832
O 1.872588 -0.208401 -1.536841
V 0.364853 0.015859 0.035080
O -1.052480 0.492730 1.634484
O -0.838769 -1.558134 -0.494943
O 1.610212 1.675158 0.800369
O -0.778685 1.382227 -1.207542
O 1.290536 -1.743798 0.948918
O -2.867738 -0.023751 -0.237475
H 1.663005 0.009634 -2.455152
H 2.391440 -1.024547 -1.554855
H -0.745626 2.344791 -1.143977
H 1.533770 -2.020590 1.840417
H -1.721821 1.112395 -1.113156
H 0.503848 -2.258619 0.647453
H -1.083444 0.019053 2.474743
H -1.942600 0.377786 1.216944
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H 2.526610 1.856883 0.557038
H 1.415002 2.189222 1.593931
H -0.774395 -1.994301 -1.352009
H -3.786306 -0.284729 -0.368485
H -2.256417 -0.819979 -0.405486

VOH+(H2O)7
E = -1554.797986
O 0.528149 -2.176145 -0.124675
V 0.499913 0.000749 0.043714
O 2.115308 0.002242 1.539103
O 0.521171 2.177312 -0.127388
O -1.142652 -0.001318 1.318334
O 2.138808 0.002539 -1.440445
O -0.994983 -0.003493 -1.543836
O -2.101010 2.045935 0.011867
O -2.095655 -2.049639 0.011090
H -0.415582 -2.472242 -0.066286
H 1.042105 -2.748432 0.457449
H -1.580492 -0.774635 -1.411107
H 3.053875 0.005882 1.311638
H -1.581801 0.767488 -1.418533
H 2.050585 0.005782 2.501823
H 1.033306 2.753273 0.452668
H -0.424065 2.469280 -0.068482
H 2.174812 -0.770306 -2.021670
H 2.173653 0.774649 -2.022695
H -1.078396 -0.001432 2.278880
H -2.891091 2.550456 0.235247
H -1.961812 1.319410 0.691628
H -2.887994 -2.552543 0.230062
H -1.958199 -1.323317 0.691566

VOH+(H2O)8
E = -1631.238884
O -0.280123 -2.092908 0.316808
V 0.726333 -0.168140 0.098232
O -0.578289 0.248111 -1.574035
O 2.192257 -0.675949 1.663859
O 1.834589 1.615985 -0.525166
O -0.542054 0.948824 1.301504
O 2.104089 -1.299421 -1.217651
O -2.598838 -1.499971 -0.848064
O -0.532334 2.808517 -0.537855
O -3.088540 0.287060 0.961837
H -1.192911 -2.083304 -0.071555
H -0.348959 -2.528277 1.175066
H -1.404908 -0.277575 -1.583324
H 2.983377 -1.199507 1.483540
H -0.836872 1.190866 -1.555856
H 2.190400 -0.467601 2.605766
H 2.580161 1.981417 -0.034272
H 1.165232 2.337797 -0.614945
H 1.783446 -2.156469 -1.531151
H 2.422793 -0.825938 -1.998843
H -0.298033 1.186871 2.202228
H -2.164676 0.563406 1.230650
H -1.001754 3.648936 -0.493712
H -0.691186 2.293646 0.309569
H -3.307376 -1.989179 -1.281842
H -3.003412 -0.898262 -0.157556
H -3.667037 0.368429 1.726999

V(OH)2+(H2O)3
E = -1324.890223
O -0.464250 -0.976378 1.508120
V 0.000295 -0.084821 0.000062
O 0.465044 -0.976741 -1.507825
O 2.123476 0.046307 0.227293
O -2.123330 0.044667 -0.227558
O -0.001350 1.985726 -0.000336
H 0.115364 -1.445383 2.121995
H 2.504271 -0.479899 -0.496204
H -2.637395 -0.141649 -1.025275
H 2.637760 -0.139535 1.024994
H -2.503450 -0.482036 0.495919
H 0.783727 2.549618 0.044773
H -0.115676 -1.446215 -2.120325
H -0.788103 2.547333 -0.044866

V(OH)2+(H2O)4
E = -1401.335139
O -0.973003 1.688607 -0.956177
V -0.396430 -0.008321 0.072834
O -2.320236 -0.814358 -0.476690
O -1.055985 -0.297619 1.735083
O 1.308399 1.118893 0.539564
O 3.221138 -0.423155 -0.156337
O 0.657698 -1.278697 -0.733665
H -0.422785 2.482924 -1.011828
H -1.828211 1.859813 -1.374087
H 2.169574 0.645089 0.285076
H -2.735808 -1.088414 0.358207
H 1.438575 1.509315 1.413459
H -2.538135 -1.478333 -1.144624
H -0.571461 -0.214640 2.566909
H 2.606972 -1.050057 -0.583879
H 3.985052 -0.306389 -0.734267
H 0.310023 -2.117301 -1.064360

V(OH)2+(H2O)5
E = -1477.780428
O 0.967674 -1.165082 -0.883872
V -0.103815 0.392636 -0.093421
O -1.705584 -0.352487 -1.234156
O 0.010645 2.071235 -0.780532
O -1.068471 0.108729 1.445496
O 3.473801 -1.196322 0.148441
O -3.308752 -1.166170 0.589890
O 1.684321 0.968857 0.947200
H 1.896344 -1.381297 -0.638870
H 0.582489 -1.851789 -1.443898
H -2.480733 -0.669129 -0.665748
H -0.680657 2.523361 -1.281031
H -2.058984 0.097797 -2.010859
H 1.864400 1.893528 0.714993
H -2.751785 -0.721681 1.262074
H -0.687756 0.363906 2.296898
H -4.232811 -0.989446 0.802941
H 4.254767 -1.065848 -0.408819
H 3.742744 -1.845622 0.814561
H 2.510659 0.465504 0.846702

V(OH)2+(H2O)6
E = -1554.223167
O -0.345855 -1.474210 1.788127
V -0.234808 -0.531387 0.231892
O 1.182345 0.898790 0.010036
O 1.274484 -1.992828 -0.221504
O -1.284087 -1.032859 -1.201464
O -3.580522 0.345488 -0.872484
O -1.628835 0.986773 0.672218
O 3.567826 -0.382946 -0.718329
O 1.081283 3.538915 0.109218
H -1.059375 -1.391684 2.433508
H 2.194616 -1.712621 -0.380562
H -2.970266 -0.290772 -1.304966
H 1.272999 -2.605929 0.530539
H -1.022716 -1.808531 -1.715676
H 2.096480 0.675489 -0.253742
H 1.078363 1.885331 0.071997
H 4.349208 -0.366994 -0.147716
H 3.912439 -0.335073 -1.621443
H -2.470689 0.901946 0.120077
H 0.559777 4.087221 -0.490515
H 1.269411 4.085188 0.882772
H -1.893145 1.176038 1.580748
H -4.049620 0.825310 -1.565076

V(OH)2+(H2O)7

E = -1630.664045
O -1.225273 0.975283 -0.900255
V 0.060203 -0.523540 0.034835
O 1.106791 1.297659 0.589000
O -1.058840 -1.793767 -0.743177
O 1.366893 -1.424403 1.021463
O -1.332348 -0.310794 1.649250
O 1.397585 -0.622841 -1.631715
O 3.422314 -0.103020 0.062076
O -3.320647 -0.673481 -0.115521
O -0.450790 3.567762 -0.023327
H -1.183004 1.912805 -0.636166
H -2.158189 0.685085 -0.852621
H 0.825307 2.211575 0.410449
H 2.077732 1.219954 0.524519
H -2.729130 -1.364940 -0.507762
H 1.170222 -2.029026 1.745729
H 1.236564 -0.116521 -2.437433
H 2.322381 -0.454312 -1.337020
H -1.213004 -0.767820 2.490618
H -2.244044 -0.497193 1.323578
H 2.949871 -0.775282 0.614589
H -0.273443 4.263461 -0.671353
H -4.238168 -0.947820 -0.227696
H 4.371908 -0.227919 0.174045
H -0.850895 4.019872 0.732493
H -0.694239 -2.389678 -1.409522

HV(OH)2+(H2O)7
E = -1631.199186
O 0.954862 -1.954109 -0.206498
V -0.402085 -0.712964 -0.310457
O 0.746216 0.708702 -1.454033
O -1.777665 -1.533112 0.351691
O 0.624454 0.335294 1.239091
O -1.687040 1.030869 -0.453504
O -4.197553 -0.043661 0.254985
O 2.957369 -1.023280 1.244393
O -0.022040 3.034309 0.703992
O 3.282343 0.833160 -0.753121
H 2.368177 -1.650594 0.754372
H 0.940274 -2.675198 -0.849402
H 1.512582 -0.001309 1.498236
H -4.827120 -0.215015 -0.459169
H 0.629332 1.310383 1.226675
H -4.737205 0.084741 1.046998
H -2.613762 0.935706 -0.166372
H -1.325269 1.872871 -0.121104
H -2.713846 -1.258719 0.386339
H 0.611945 0.600755 -2.403470
H 1.733191 0.719065 -1.285099
H -0.236615 3.710441 1.361047
H 0.546320 3.474024 0.056337
H 3.453603 -1.523910 1.902856
H 4.065893 0.911727 -1.309682
H 3.475475 0.157265 -0.070785
H -0.682597 -1.159429 -1.843222

IR frequencies (in cm^{-1}, without shift) and intensities (KM/mole) for optimized structures

IIIa
29.2116 6.63
100.4123 27.9613
115.6578 9.0529
127.5987 0.7713
154.9182 101.0679
256.4148 0.8872
294.7278 69.7465
298.7716 0.0317
321.5702 23.7717
327.5694 157.8457
378.3872 83.5792
383.6366 135.821
471.6229 1.6006
497.5826 6.6675
500.6928 60.2387
1620.7903 158.5086
1626.4813 84.0752
1629.1639 117.9509
3742.5625 40.9156
3747.7323 61.9026
3769.9117 57.4104
3831.2512 138.508
3836.5109 177.7459
3871.9189 166.1723

IVa
44.4627 18.2648
48.6768 109.8995
61.1796 10.3131
72.0393 0.0327
94.0252 2.1339
120.9735 2.0443
135.6046 22.9128
152.6394 147.0518
171.3094 0.9112
217.0438 156.071
261.265 0.0692
268.7703 1.4151
285.5793 3.6592
320.4889 131.5965
331.2421 15.814
337.8662 37.1394
365.5608 172.8243
434.9625 0.0166
449.9725 0.0048
475.7373 0.0061
484.9311 48.9199
1615.4008 220.4813
1616.6203 45.151
1621.2947 131.8713
1625.0472 97.8528
3741.77 12.7396
3743.3627 12.5991
3757.5923 9.5001
3783.3327 52.3216
3835.5795 71.8137
3837.8748 136.7695
3852.0875 151.3951
3879.8655 134.8443

iIVa
87.097 0.1598
108.3064 3.2887
137.1009 6.1011
144.2954 7.0902
160.8182 18.435
213.4439 12.3564
244.3739 19.1611
320.9888 0.403
350.9581 146.9492
353.1423 30.2364
376.2187 9.6924
378.3559 82.8932
416.4697 203.2819
435.3377 163.6432
476.8875 120.2836
519.3671 100.4495
553.8967 149.985
566.3846 58.2565
579.2894 23.1244
634.4703 60.9039
691.6552 109.8973
760.1307 172.994
1620.7659 141.3335
1622.5389 11.6725
1625.1262 177.8241
1769.6226 181.9254
3716.7458 91.6611
3744.1504 95.8676
3749.2419 119.1102
3805.3278 104.0659
3817.4222 166.3532
3834.5071 161.8393
3843.816 193.5232

Va
32.9237 28.2167
45.2402 3.882
78.2181 0.3473
81.1911 0.2342
81.5809 16.3737
95.7964 2.1454
135.1324 4.2821
144.2206 32.1887
145.5624 2.7033
204.8959 1.5774
209.7341 34.4339
217.3749 20.4595
233.4548 314.7104
257.262 101.6293
276.8767 0.1047
288.3653 5.5347
290.1779 1.5139
316.8508 25.6155
355.3681 43.6392
355.6662 11.0391
433.0625 110.9896
441.8084 0.0736
444.1005 2.2618
556.8325 115.6597
616.7921 98.3348
619.7621 30.9262
672.1362 90.2829
1606.5089 92.2991
1609.8244 91.1149
1610.97 210.1004
1617.4893 101.7377
1655.6766 4.2414
3610.4294 71.5625
3641.4229 804.7842
3737.7826 3.5817
3738.21 5.2395
3764.5485 15.5152
3833.9546 1.2542
3835.4902 213.4392

3854.5208 196.3706
3856.2098 92.0926
3857.4376 124.9999

Vb
21.6662 0.28
35.8649 11.4231
45.3816 14.8264
60.5851 3.5889
81.8556 2.2224
87.0322 6.3781
103.5745 3.3766
129.0041 83.894
135.1881 25.9489
144.4401 43.0649
144.7843 108.0253
208.0118 35.1177
220.7977 18.2062
273.3446 50.0383
279.3072 51.9767
291.6335 54.6325
296.9954 26.7893
318.4296 200.9197
333.0714 65.4282
351.226 71.4166
354.389 127.8514
375.6288 13.8073
459.213 8.3538
480.7629 1.9727
499.4348 37.1697
570.3715 23.977
841.763 90.6142
1612.2047 137.4586
1621.5211 162.4664
1623.2223 55.974
1623.9774 31.9953
1644.5413 98.5472
3382.6882 1115.2107
3735.1923 7.2919
3749.6183 15.7497
3755.5025 19.9802
3792.6414 34.8981
3818.5699 74.0355
3831.2887 114.3775
3844.5228 115.6927
3850.3409 111.0474
3894.9577 117.3446

Vc
18.7748 2.7385
32.7532 4.7276
44.8587 1.5019
51.2566 1.911
66.096 2.1835
94.4042 4.3704
102.5563 12.1973
123.9884 52.6301
130.4916 17.9298
138.5002 40.8467
145.0484 123.8932
204.7683 212.4798
231.0696 28.5659
245.0419 27.9977
271.0396 2.814
297.8225 4.8116
308.3309 11.3953
322.6747 103.8551
337.2626 86.2302
363.6326 153.7401
387.0562 62.5897
438.5907 16.7959
468.3519 1.2188
618.8253 7.3703
630.1283 29.8597
823.0012 68.6093
884.4896 84.0305
1616.2812 107.2775
1618.5624 175.2674
1619.1637 63.3799
1642.3329 48.0606
1649.868 25.2816
3287.0869 1347.831
3389.5181 1352.4732
3745.9884 31.5181
3790.452 35.4664
3791.5513 39.53
3813.9911 95.8137
3828.7162 88.8254
3838.8498 126.7149
3892.501 118.2542
3894.6214 127.3752

iVa
38.3333 1.2881
49.7487 1.2891
92.7497 5.4058
113.4515 4.5279
128.9751 5.3963
142.5947 5.8748
152.0293 5.3223
170.4208 16.244
185.6586 179.5454
212.7936 4.8591
247.442 94.7223
268.1313 38.607
316.1228 0.1836
346.876 7.6371
373.8642 17.1035
396.473 66.08
413.8249 258.2565
432.0766 151.7773
459.8412 76.3812
473.6199 100.1538
516.4997 113.415
564.9828 93.5939
581.3717 4.5567
637.8671 32.0216
691.3742 112.6218
711.2859 69.7966
752.199 174.9349
961.4099 99.9182
1614.1757 123.608
1618.5005 21.0648
1618.9856 168.1235
1649.1354 40.0594
1755.0419 207.6862
3111.8835 1957.4626
3717.6891 78.1272
3748.2457 78.7949
3786.3997 49.4949
3815.3307 95.0964
3817.1684 127.4316
3829.0125 152.1785
3840.2396 153.3302
3887.2559 144.1114

iVb
43.9311 8.8577
81.7001 0.3322
113.8155 1.0327
118.811 12.0222
144.0091 3.9438
152.3304 1.6531
201.3793 59.1476
222.1512 9.6143
258.7883 82.7451
310.9854 50.6202
322.1758 109.8984
325.8906 71.8592
354.504 8.2128

375.0091 36.9845
392.8141 20.9835
403.0573 228.92
411.0561 68.8154
428.8181 77.0437
454.1063 126.2364
504.2976 11.9609
530.2392 126.142
546.6208 87.8144
565.128 58.746
630.0512 111.5075
699.0425 90.3273
719.7776 220.1977
752.6026 64.3111
1022.6555 111.0151
1585.8614 92.6458
1613.604 109.786
1617.4368 132.6125
1658.0016 59.4785
1766.3108 179.3265
2946.0426 1414.5904
3667.9815 201.0837
3748.6372 94.0194
3751.8851 113.206
3804.7599 91.7641
3810.6042 128.9756
3841.8322 151.1002
3851.424 185.8704
3862.3842 188.4397

iVc
45.1119 7.4196
46.9501 7.5401
92.569 53.0734
106.2222 9.4026
140.1239 2.2818
155.346 11.0546
171.1927 15.4665
197.0965 28.3468
223.1678 95.1071
254.7795 20.4217
284.6533 26.2249
298.5148 93.7013
319.2189 89.7448
331.517 242.2255
347.2029 46.1416
368.9169 15.5501
382.8287 27.5099
411.9729 297.0964
437.2261 6.8173
484.2434 98.9121
505.5352 78.8891
534.5301 114.2556
565.2844 31.6343
605.5337 28.0313
688.6908 195.2855
697.1692 139.0004
722.7203 47.0219
1004.2316 115.8521
1577.0744 97.9214
1607.8119 127.716
1616.2718 119.2332
1646.3262 74.3919
1755.4375 177.8988
2975.3818 1393.527
3701.3635 121.3952
3756.0221 94.394
3762.716 107.1008
3797.2766 123.8363
3817.4332 141.4961
3852.3884 157.4435
3862.7875 170.4785
3869.1162 192.7617

VIa
23.7803 1.6819
36.2283 1.1314
55.668 11.6028
69.3366 0.2602
79.1236 0.1406
91.5242 0.005
93.9687 3.042
98.0657 11.1213
108.1642 32.7231
127.3656 120.0966
143.522 59.7691
153.6604 45.9929
174.8071 1.847
205.7425 64.2545
207.0362 122.7595
229.215 108.8974
232.3448 234.6862
278.8178 1.4162
288.6414 6.706
293.8644 30.7402
303.0003 31.6125
307.1226 9.8339
358.7482 43.5765
363.0474 8.6022
392.314 17.9595
427.723 3.6858
436.0404 3.3797
436.1651 0.4862
591.8377 77.9827
656.329 125.0418
660.9725 10.2611
777.273 78.1911
903.2662 94.7481
1603.1706 81.1385
1607.5357 202.0287
1610.3229 91.0929
1621.8556 94.1909
1628.3804 36.7709
1670.642 13.1255
3398.8988 1582.1759
3482.6994 144.116
3547.5435 760.9129
3735.71 8.2755
3736.0779 1.411
3794.4284 32.1325
3833.2941 0.0287
3834.1171 63.9927
3834.7469 223.415
3855.1043 171.7601
3856.0068 61.8886
3896.8222 119.2295

VIb
11.8195 0.2839
30.1653 6.9128
39.6496 7.8205
67.5391 5.5572
77.1071 7.8788
83.9911 1.6781
93.118 2.2503
115.0158 12.9161
126.9412 12.5495
131.955 8.1634
146.6623 3.137
159.8675 56.2277
209.7195 23.8758
210.901 48.0604
217.424 18.9233
226.8052 87.942
246.6378 63.0881
264.4743 199.6587
277.9527 6.6119
280.3146 5.3879
301.6642 106.5802
311.3797 4.8498

335.3601 76.034
350.1947 14.5621
376.1232 49.0046
426.1438 116.0321
445.6556 4.3922
537.0726 78.7887
592.1063 136.9569
601.4648 14.6198
626.4354 41.8101
680.1253 64.2015
739.8513 71.6463
1602.6884 141.2648
1605.7475 81.459
1615.8261 125.8831
1622.8813 98.8092
1651.0203 10.9336
1653.2152 61.2325
3421.9971 897.4996
3619.3969 69.5829
3647.2058 681.2575
3725.6285 10.3824
3765.1274 12.2985
3785.7309 23.1531
3818.9413 68.2359
3824.1495 105.7356
3846.3932 146.3859
3851.8945 131.7843
3859.2292 117.9671
3886.9523 107.1743

iVIa
32.1944 6.8225
55.2065 1.5771
93.495 0.4553
93.9865 0.3114
130.5842 2.5289
138.6049 2.778
155.7363 1.0915
165.9196 1.3104
218.2973 77.2433
240.0969 19.1781
254.2858 34.8168
278.2301 56.9201
298.0415 23.3485
314.2148 74.2958
328.76 84.8735
336.7782 19.8731
363.1573 64.1237
394.8108 41.0072
403.5772 23.4222
421.4414 41.4927
446.5793 210.5184
467.4763 104.3309
483.5944 69.0686
522.9733 17.4871
553.4829 111.2266
588.3446 96.0895
596.7959 45.6064
663.6662 175.153
695.0132 80.3332
717.0352 78.4774
736.0111 166.985
779.5661 113.6259
794.9983 192.4302
1021.3076 106.3065
1592.6977 89.4297
1599.672 110.7595
1622.8289 112.6956
1655.0699 29.2853
1664.4369 51.3179
1757.8149 202.9634
2972.8025 1335.4955
3450.0437 734.9057
3606.6225 370.8213
3639.4705 482.1564
3756.3026 36.0231
3794.6512 88.0034
3817.2339 120.3338
3819.2987 232.7647
3825.0487 142.8995
3845.2693 146.7256
3860.2157 163.4348

VIIIa
9.4753 2.3495
27.1885 2.721
27.8463 0.0411
36.0862 0.2255
43.617 4.5563
72.2596 0.1306
76.0583 3.1388
81.1432 0.6452
88.6541 2.7146
93.7257 0.9765
94.4083 4.6185
122.0332 145.7625
129.6427 65.8024
137.4448 63.1863
145.0539 208.3711
157.8576 0.1281
173.9422 0.2146
187.5461 23.0832
202.3764 61.6703
231.9433 0.1193
253.4314 5.4893
280.5952 96.0711
286.0396 9.2735
286.1451 0.5452
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VIIIb
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IXd
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3809.9341 26.3284
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3813.4781 284.3108
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3900.174 105.5592

IXe
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201.0174 178.3619
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iIXa
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iIXb
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