

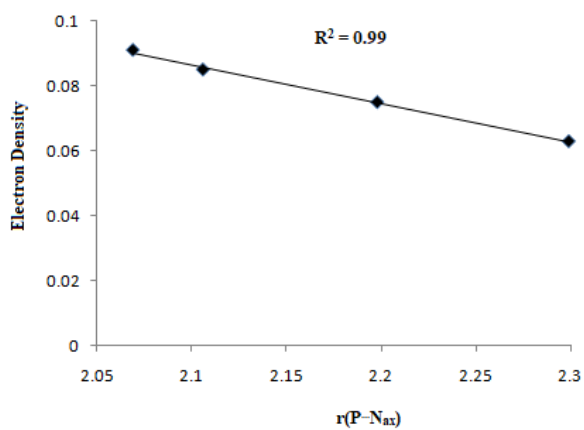
Supporting Information of

Protonation of Verkade Bases: A Theoretical Study

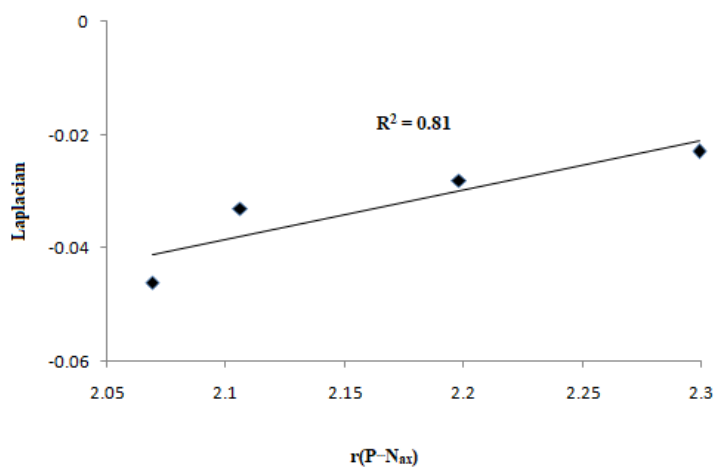
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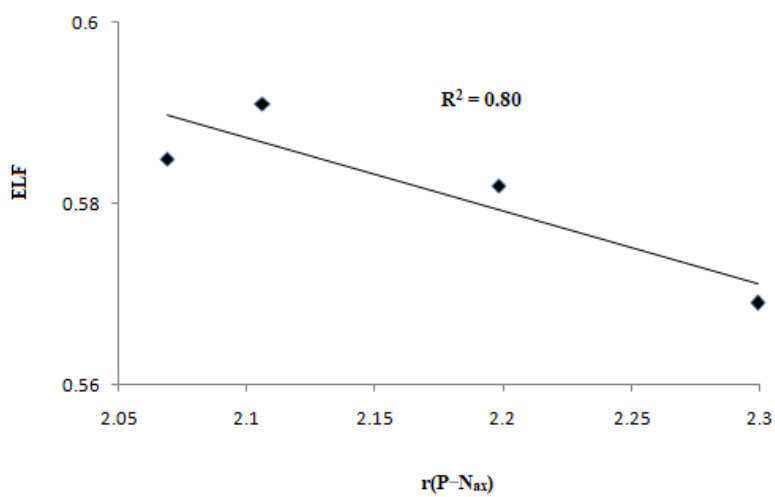
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(a)



(b)



(c)

Fig S1. Variation of P...Nax distance (Å) against (a) electron density at the bond critical point (b) laplacian of electron density and (c) electron localization function.

Cartesian coordinates of the optimized geometries along with the energies in a.u.

1

Sum of electronic and zero-point Energies = -797.720390
Sum of electronic and thermal Energies = -797.710177
Sum of electronic and thermal Enthalpies = -797.709233
Sum of electronic and thermal Free Energies = -797.754672

15	0.000000	0.000000	0.000000
7	0.000000	0.000000	1.725288
1	0.954027	0.000000	2.056401
7	-0.956764	-1.382606	-0.386455
1	-0.450971	-1.962716	-1.040110
7	-1.047328	1.315883	-0.387225
1	-0.556815	1.962655	-0.987873
6	-0.857175	-0.848953	2.551956
1	-0.904364	-1.867356	2.145743
1	-0.419096	-0.908366	3.552378
6	-2.275691	-0.292148	2.661627
1	-2.869336	-0.972349	3.292302
1	-2.240924	0.675376	3.170978
6	-1.888359	2.015148	0.584212
1	-1.339477	2.191635	1.518010
1	-2.158443	2.989122	0.166140
6	-3.164505	1.235795	0.898963
1	-3.767419	1.156042	-0.010371
1	-3.752509	1.810464	1.631610
6	-2.385004	-1.337999	-0.698799
1	-2.613558	-0.488007	-1.354022
1	-2.647808	-2.253973	-1.235664
6	-3.241551	-1.236023	0.562188
1	-4.300820	-1.205850	0.262493
1	-3.099679	-2.138556	1.163631
7	-2.911619	-0.098135	1.382793

1-H⁺ (P protonated)

Sum of electronic and zero-point Energies= -798.107697
Sum of electronic and thermal Energies= -798.097524
Sum of electronic and thermal Enthalpies= -798.096579
Sum of electronic and thermal Free Energies= -798.142321

15	-0.040817000	-0.866803000	-0.821829000
7	0.913179000	-1.678533000	0.298792000
1	1.288399000	-2.557603000	-0.034980000
7	-1.687148000	-0.866095000	-0.624910000
1	-2.223402000	-1.412719000	-1.283225000
7	0.735284000	0.336707000	-1.674502000

1	1.011177000	0.139105000	-2.624995000
6	1.866734000	-0.846201000	1.026951000
1	2.326289000	-1.424386000	1.827293000
1	2.661219000	-0.473747000	0.370484000
6	1.052990000	0.313070000	1.612900000
1	0.658191000	0.040957000	2.590294000
1	1.659786000	1.211416000	1.729307000
6	1.038654000	1.650342000	-1.123791000
1	2.060339000	1.695164000	-0.732757000
1	0.935123000	2.417398000	-1.891273000
6	0.016889000	1.872289000	-0.016733000
1	-0.953924000	2.098301000	-0.459631000
1	0.293099000	2.678412000	0.665675000
6	-2.407006000	0.032035000	0.263298000
1	-2.777623000	0.912974000	-0.269537000
1	-3.263260000	-0.478725000	0.704336000
6	-1.412568000	0.396422000	1.355914000
1	-1.701967000	1.290012000	1.914024000
1	-1.315235000	-0.445134000	2.041245000
7	-0.095599000	0.584530000	0.703244000
1	-0.040126000	-1.833386000	-1.848425000

1-H⁺ (N_{eq} protonated)

Sum of electronic and zero-point Energies=	-798.084533
Sum of electronic and thermal Energies=	-798.073882
Sum of electronic and thermal Enthalpies=	-798.072938
Sum of electronic and thermal Free Energies=	-798.119639

15	-0.617063000	-1.593269000	-0.155418000
7	0.679758000	-1.241043000	1.331864000
1	0.970273000	-2.170078000	1.640662000
7	-1.833143000	-0.572312000	0.358175000
1	-2.666001000	-1.118651000	0.542776000
7	0.243772000	-1.048044000	-1.471304000
1	0.417758000	-1.841333000	-2.078401000
6	1.886254000	-0.395596000	1.094294000
1	2.589812000	-0.531539000	1.917971000
1	2.351543000	-0.767339000	0.182156000
6	1.454802000	1.072244000	0.979871000
1	1.241410000	1.455044000	1.981861000
1	2.297592000	1.657633000	0.592227000
6	0.956004000	0.153486000	-1.944138000
1	2.030608000	0.020404000	-1.786778000
1	0.798649000	0.238010000	-3.020995000
6	0.476642000	1.426968000	-1.259552000
1	-0.471907000	1.736878000	-1.698806000
1	1.200357000	2.229581000	-1.456634000
6	-2.111972000	0.859513000	0.182385000
1	-2.294899000	1.078881000	-0.873570000

1	-3.030611000	1.090326000	0.723124000
6	-0.963026000	1.700892000	0.721277000
1	-1.142910000	2.761169000	0.497990000
1	-0.920268000	1.594188000	1.807745000
7	0.278162000	1.205699000	0.156603000
1	0.112464000	-0.849277000	2.087756000

1-H⁺ (Nax protonated)

Sum of electronic and zero-point Energies=	-798.067197
Sum of electronic and thermal Energies=	-798.056759
Sum of electronic and thermal Enthalpies=	-798.055815
Sum of electronic and thermal Free Energies=	-798.101742

15	1.655971000	0.718394000	-0.141713000
7	1.600763000	-0.888808000	-0.702595000
1	2.496269000	-1.211726000	-1.037746000
7	0.301332000	1.455322000	-0.951052000
1	0.612451000	2.119305000	-1.646491000
7	0.935451000	0.590422000	1.426671000
1	1.548897000	0.953665000	2.143497000
6	0.530440000	-1.851514000	-0.896157000
1	0.755492000	-2.433327000	-1.795153000
1	0.456987000	-2.581252000	-0.081526000
6	-0.840492000	-1.270741000	-1.189529000
1	-0.768930000	-0.541589000	-1.990744000
1	-1.481785000	-2.095999000	-1.501607000
6	0.270991000	-0.627587000	1.844589000
1	0.840248000	-1.516428000	1.569472000
1	0.208131000	-0.632580000	2.935942000
6	-1.193192000	-0.763619000	1.410608000
1	-1.804471000	-0.038316000	1.950181000
1	-1.529619000	-1.765572000	1.685422000
6	-0.909869000	1.871763000	-0.269146000
1	-0.720284000	2.070846000	0.787898000
1	-1.289240000	2.793670000	-0.714505000
6	-2.021889000	0.844801000	-0.401655000
1	-2.856562000	1.092107000	0.258241000
1	-2.391100000	0.788491000	-1.426797000
7	-1.612115000	-0.576477000	-0.050043000
1	-2.510003000	-1.059008000	-0.063510000

TS (proton transfer from P to Neq in 1)

Sum of electronic and zero-point Energies=	-797.998249
Sum of electronic and thermal Energies=	-797.987623
Sum of electronic and thermal Enthalpies=	-797.986679
Sum of electronic and thermal Free Energies=	-798.034380

15	-0.774405000	-1.269541000	-0.322359000
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7	-1.192587000	-0.141101000	-1.541627000
7	0.796235000	-1.777374000	-0.450070000
7	-1.345676000	-0.740252000	1.190775000
6	-1.057689000	1.370781000	-1.349132000
1	-1.223190000	1.812954000	-2.328291000
1	-1.840945000	1.730853000	-0.676821000
6	0.285912000	1.882628000	-0.844246000
1	1.006260000	1.919562000	-1.660584000
1	0.176546000	2.926042000	-0.500389000
6	-1.034752000	0.533333000	1.847057000
1	-1.810424000	1.240232000	1.539064000
1	-1.110712000	0.375916000	2.929880000
6	0.360598000	1.135869000	1.551113000
1	1.146257000	0.736518000	2.200535000
1	0.259815000	2.191750000	1.843260000
6	2.053549000	-1.089589000	-0.006293000
1	2.214576000	-1.337829000	1.050521000
1	2.881042000	-1.503819000	-0.587009000
6	2.099060000	0.423786000	-0.134548000
1	2.911538000	0.791181000	0.514529000
1	2.367361000	0.721843000	-1.148600000
7	0.791486000	0.982336000	0.164815000
1	-2.351565000	-0.970207000	1.239845000
1	0.870656000	-2.774230000	-0.179769000
1	-2.174598000	-0.234466000	-1.824667000
1	-1.292810000	-2.389294000	0.492908000

2

Sum of electronic and zero-point Energies=	-915.500006
Sum of electronic and thermal Energies=	-915.484864
Sum of electronic and thermal Enthalpies=	-915.483920
Sum of electronic and thermal Free Energies=	-915.541427

15	0.607001000	0.935388000	0.605325000
7	-0.510646000	-0.029385000	1.524169000
7	1.794853000	-0.211561000	0.157208000
7	-0.254696000	1.455190000	-0.796758000
6	-1.878184000	-0.203396000	1.059492000
1	-2.515567000	-0.414375000	1.923094000
1	-2.270266000	0.714930000	0.602808000
6	-1.956189000	-1.391269000	0.074034000
1	-2.042805000	-2.316890000	0.650842000
1	-2.865468000	-1.315371000	-0.535492000
6	-1.067941000	0.754336000	-1.785250000
1	-2.135935000	0.863349000	-1.538637000
1	-0.931914000	1.257227000	-2.751999000
6	-0.754505000	-0.724210000	-1.988668000
1	0.236902000	-0.821048000	-2.432765000
1	-1.471605000	-1.096486000	-2.738557000

6	1.679793000	-1.519263000	-0.472288000
1	1.933327000	-1.435453000	-1.540993000
1	2.449782000	-2.172119000	-0.040421000
6	0.347812000	-2.238586000	-0.312420000
1	0.454892000	-3.204808000	-0.833209000
1	0.194382000	-2.450032000	0.746112000
7	-0.805653000	-1.504496000	-0.782729000
6	-0.599330000	2.873854000	-0.784424000
1	-1.651075000	3.036898000	-0.505906000
1	0.030778000	3.408283000	-0.073707000
1	-0.445655000	3.306478000	-1.779200000
6	-0.365108000	0.148824000	2.964133000
1	-0.851856000	1.061322000	3.338786000
1	-0.790991000	-0.711982000	3.487199000
1	0.694126000	0.199567000	3.222551000
6	3.092262000	0.381313000	-0.144332000
1	3.210656000	1.319594000	0.398628000
1	3.890868000	-0.301266000	0.164359000
1	3.213723000	0.583504000	-1.218259000

2-H⁺ (P protonated)

Sum of electronic and zero-point Energies=	-915.911176
Sum of electronic and thermal Energies=	-915.896365
Sum of electronic and thermal Enthalpies=	-915.895421
Sum of electronic and thermal Free Energies=	-915.952014

15	0.003444000	-0.708295000	0.060041000
7	-0.941316000	-0.623516000	-1.345046000
7	1.664554000	-0.785191000	-0.088871000
7	-0.736416000	-0.212626000	1.486098000
6	-1.796204000	0.554639000	-1.387302000
1	-2.255053000	0.636556000	-2.373355000
1	-2.605630000	0.488136000	-0.645621000
6	-0.898365000	1.766794000	-1.121947000
1	-0.506737000	2.163983000	-2.057005000
1	-1.437126000	2.566228000	-0.613384000
6	-0.843926000	1.194908000	1.831954000
1	-1.837466000	1.589559000	1.579127000
1	-0.700679000	1.326732000	2.907403000
6	0.253474000	1.912928000	1.064667000
1	1.219873000	1.705510000	1.525810000
1	0.107076000	2.993535000	1.014553000
6	2.470721000	0.394232000	-0.350832000
1	2.940006000	0.759122000	0.571619000
1	3.274830000	0.144953000	-1.047534000
6	1.550850000	1.424554000	-0.981992000
1	1.942923000	2.442425000	-0.919008000
1	1.380056000	1.163663000	-2.026104000
7	0.250019000	1.316426000	-0.287621000

1	-0.147406000	-2.087755000	0.301079000
6	-1.595521000	-1.855115000	-1.792232000
1	-1.934884000	-1.717988000	-2.819431000
1	-0.883592000	-2.679778000	-1.786502000
1	-2.458644000	-2.120243000	-1.168813000
6	2.427535000	-1.938646000	0.385411000
1	2.952301000	-1.700452000	1.315487000
1	1.771523000	-2.788534000	0.566168000
1	3.160089000	-2.228525000	-0.370621000
6	-1.603613000	-1.102789000	2.254842000
1	-1.364665000	-1.026032000	3.317879000
1	-2.657650000	-0.843219000	2.111450000
1	-1.458391000	-2.138145000	1.948872000

2-H⁺ (N_{eq} protonated)

Sum of electronic and zero-point Energies=	-915.891466
Sum of electronic and thermal Energies=	-915.875891
Sum of electronic and thermal Enthalpies=	-915.874946
Sum of electronic and thermal Free Energies=	-915.933458

15	0.272411000	-0.901146000	0.985639000
7	-1.281277000	-1.227391000	0.512790000
7	1.416126000	-0.847843000	-0.957757000
7	0.388954000	0.660613000	1.510974000
6	-2.366339000	-0.353181000	0.035569000
1	-3.223213000	-0.991435000	-0.186880000
1	-2.689402000	0.314625000	0.830758000
6	-1.977316000	0.426025000	-1.225732000
1	-1.899247000	-0.275369000	-2.059740000
1	-2.787658000	1.130826000	-1.463905000
6	-0.531478000	1.786395000	1.316720000
1	-1.502782000	1.538685000	1.739105000
1	-0.152496000	2.624668000	1.904093000
6	-0.637670000	2.210158000	-0.160141000
1	0.247979000	2.797556000	-0.415052000
1	-1.506658000	2.872937000	-0.276414000
6	1.612709000	0.481155000	-1.561437000
1	2.003186000	1.139017000	-0.777595000
1	2.362756000	0.430323000	-2.358463000
6	0.293679000	1.019768000	-2.103512000
1	0.471853000	1.998251000	-2.566695000
1	-0.062673000	0.360300000	-2.899876000
7	-0.701756000	1.078100000	-1.055946000
1	0.869367000	-1.424564000	-1.597775000
6	-1.555087000	-2.663271000	0.310863000
1	-1.738606000	-2.874423000	-0.746540000
1	-0.710199000	-3.265216000	0.648648000
1	-2.432139000	-2.955311000	0.890249000
6	2.688530000	-1.526314000	-0.657681000

1	3.252594000	-0.913574000	0.048250000
1	2.489670000	-2.492226000	-0.193818000
1	3.289205000	-1.668321000	-1.558576000
6	1.639616000	0.998800000	2.211713000
1	1.413982000	1.383619000	3.207740000
1	2.263678000	0.110770000	2.324399000
1	2.200451000	1.754484000	1.654902000

2-H⁺ (N_{ax} protonated)

Sum of electronic and zero-point Energies=	-915.866043
Sum of electronic and thermal Energies=	-915.850988
Sum of electronic and thermal Enthalpies=	-915.850044
Sum of electronic and thermal Free Energies=	-915.906682

15	1.021337000	0.201869000	0.985659000
7	1.204640000	1.195898000	-0.405059000
7	-0.639221000	0.471431000	1.370596000
7	0.853790000	-1.416231000	0.377739000
6	0.356007000	1.362696000	-1.569477000
1	0.435266000	2.412865000	-1.882488000
1	0.711570000	0.783241000	-2.433974000
6	-1.138582000	1.170631000	-1.401878000
1	-1.504079000	1.760365000	-0.566666000
1	-1.604476000	1.538902000	-2.317536000
6	0.608913000	-1.595018000	-1.038821000
1	1.273654000	-0.977841000	-1.649165000
1	0.852249000	-2.631136000	-1.296796000
6	-0.842990000	-1.472761000	-1.521030000
1	-1.427781000	-2.306153000	-1.127975000
1	-0.829950000	-1.552400000	-2.610236000
6	-1.669540000	-0.530490000	1.297391000
1	-1.221542000	-1.524641000	1.309995000
1	-2.334401000	-0.455250000	2.164636000
6	-2.532166000	-0.381778000	0.051433000
1	-3.178765000	-1.250830000	-0.089393000
1	-3.157537000	0.512145000	0.087068000
7	-1.705055000	-0.246968000	-1.214268000
6	2.563798000	1.671089000	-0.672527000
1	3.167220000	1.585050000	0.231044000
1	3.050569000	1.094469000	-1.469078000
1	2.541381000	2.722718000	-0.972654000
6	1.831226000	-2.372834000	0.919495000
1	1.429664000	-3.386046000	0.849710000
1	2.791352000	-2.335282000	0.390960000
1	2.010690000	-2.153286000	1.971297000
6	-0.969751000	1.699786000	2.078945000
1	-1.726859000	2.293374000	1.549413000
1	-1.345102000	1.489078000	3.085289000
1	-0.078673000	2.323476000	2.170902000

1 -2.415079000 -0.307704000 -1.943499000

TS (proton transfer from P to N_{eq} in 2)

Sum of electronic and zero-point Energies= -915.771915
Sum of electronic and thermal Energies= -915.759167
Sum of electronic and thermal Enthalpies= -915.758223
Sum of electronic and thermal Free Energies= -915.809933

15 0.352852000 0.974705000 -0.312063000
7 1.032966000 -0.177817000 -1.381644000
7 -1.246717000 1.258837000 -0.631066000
7 0.824306000 0.642345000 1.288980000
6 1.067554000 -1.675193000 -1.069064000
1 1.388022000 -2.164710000 -1.985215000
1 1.814957000 -1.876178000 -0.296965000
6 -0.247378000 -2.320607000 -0.648879000
1 -0.868356000 -2.514590000 -1.522624000
1 -0.045759000 -3.311149000 -0.204934000
6 0.607176000 -0.607581000 2.023786000
1 1.492532000 -1.226867000 1.853901000
1 0.549515000 -0.359615000 3.090672000
6 -0.663938000 -1.410366000 1.653058000
1 -1.556597000 -1.070382000 2.187904000
1 -0.463840000 -2.418298000 2.046029000
6 -2.448271000 0.446332000 -0.247755000
1 -2.748343000 0.750688000 0.763053000
1 -3.255616000 0.701944000 -0.937986000
6 -2.291805000 -1.065070000 -0.244726000
1 -3.115652000 -1.486415000 0.355396000
1 -2.413648000 -1.472272000 -1.248950000
7 -0.963439000 -1.421115000 0.224337000
1 0.640174000 2.211976000 0.445472000
6 2.188810000 1.160641000 1.463331000
1 2.711692000 1.238710000 0.503327000
1 2.181794000 2.158068000 1.917421000
1 2.784097000 0.507206000 2.111224000
6 -1.566801000 2.672519000 -0.386218000
1 -0.708133000 3.209251000 0.032968000
1 -1.854767000 3.182660000 -1.312468000
1 -2.398156000 2.776844000 0.320234000
6 2.446686000 0.109835000 -1.663698000
1 2.652005000 0.084580000 -2.739948000
1 2.733057000 1.101841000 -1.296243000
1 3.106224000 -0.622675000 -1.184587000

3

Sum of electronic and zero-point Energies= -857.383754
Sum of electronic and thermal Energies= -857.373910

Sum of electronic and thermal Enthalpies= -857.372966
Sum of electronic and thermal Free Energies= -857.418507

15	1.627430000	0.520793000	-0.112437000
8	1.384379000	-0.955391000	-0.776440000
8	0.536221000	1.514334000	-0.857695000
8	0.934416000	0.400214000	1.388692000
6	0.318410000	-1.885487000	-0.951728000
1	0.548296000	-2.440255000	-1.864307000
1	0.344988000	-2.599144000	-0.124492000
6	-1.075313000	-1.281478000	-1.090639000
1	-1.143059000	-0.775663000	-2.054620000
1	-1.772141000	-2.136708000	-1.117630000
6	0.149475000	-0.684821000	1.860173000
1	0.652740000	-1.623343000	1.619969000
1	0.126289000	-0.597142000	2.948405000
6	-1.297072000	-0.662329000	1.322025000
1	-1.866611000	0.076135000	1.893952000
1	-1.745208000	-1.644793000	1.533924000
6	-0.654376000	2.010213000	-0.259910000
1	-0.483288000	2.202761000	0.802463000
1	-0.885416000	2.955799000	-0.754575000
6	-1.795450000	1.015889000	-0.443544000
1	-2.660806000	1.359395000	0.139068000
1	-2.098671000	1.009773000	-1.492667000
7	-1.448964000	-0.334840000	-0.071093000

3-H⁺ (P protonated)

Sum of electronic and zero-point Energies= -857.751551
Sum of electronic and thermal Energies= -857.742136
Sum of electronic and thermal Enthalpies= -857.741191
Sum of electronic and thermal Free Energies= -857.786029

15	-0.029397000	-1.210409000	-0.203254000
8	1.021766000	-1.237846000	0.995538000
8	-1.592847000	-1.126747000	0.072959000
8	0.543196000	-0.690721000	-1.596240000
6	1.889687000	-0.125045000	1.225965000
1	2.351338000	-0.284012000	2.196994000
1	2.666903000	-0.130266000	0.459269000
6	1.048425000	1.159244000	1.197936000
1	0.669261000	1.381121000	2.193798000
1	1.645680000	2.009843000	0.865815000
6	0.928555000	0.665173000	-1.858692000
1	1.982692000	0.781371000	-1.599773000
1	0.804815000	0.828534000	-2.926664000
6	0.025675000	1.569153000	-1.031966000
1	-0.964905000	1.607924000	-1.487308000
1	0.416153000	2.586188000	-0.958877000

6	-2.336918000	0.084254000	0.234696000
1	-2.678752000	0.407258000	-0.750187000
1	-3.202119000	-0.153299000	0.849233000
6	-1.422441000	1.091433000	0.913570000
1	-1.796249000	2.113870000	0.822198000
1	-1.331142000	0.837256000	1.969353000
7	-0.095332000	0.930414000	0.290365000
1	-0.030217000	-2.565322000	-0.484720000

3-H⁺ (N_{eq} protonated)

Sum of electronic and zero-point Energies=	-857.707313
Sum of electronic and thermal Energies=	-857.696562
Sum of electronic and thermal Enthalpies=	-857.695617
Sum of electronic and thermal Free Energies=	-857.742935

15	-1.340545000	-1.127658000	0.132002000
8	0.019988000	-1.663668000	0.700168000
8	-1.727737000	0.306190000	0.650467000
8	-0.597963000	-0.425757000	-1.673085000
6	1.383159000	-1.358216000	1.079115000
1	1.553874000	-1.877748000	2.020892000
1	2.008145000	-1.821619000	0.316015000
6	1.635863000	0.143164000	1.215651000
1	1.311459000	0.466202000	2.204419000
1	2.722462000	0.300080000	1.160734000
6	0.837766000	-0.300371000	-1.927051000
1	1.308180000	-1.238519000	-1.633217000
1	0.970312000	-0.154743000	-2.999704000
6	1.358464000	0.903065000	-1.141923000
1	1.005746000	1.814697000	-1.630547000
1	2.454590000	0.898732000	-1.216611000
6	-1.401557000	1.668994000	0.288908000
1	-1.563728000	1.763830000	-0.785959000
1	-2.117912000	2.293177000	0.819355000
6	0.036361000	1.974246000	0.674009000
1	0.315058000	2.946972000	0.251426000
1	0.106744000	2.062210000	1.758280000
7	0.917297000	0.913889000	0.231365000
1	-1.042475000	-0.855042000	-2.417329000

3-H⁺ (N_{ax} protonated)

Sum of electronic and zero-point Energies=	-857.720091
Sum of electronic and thermal Energies=	-857.710274
Sum of electronic and thermal Enthalpies=	-857.709330
Sum of electronic and thermal Free Energies=	-857.754631

15	-1.640192000	0.754736000	0.009575000
8	-0.456523000	0.986749000	-1.154089000

8	-1.874228000	-0.816266000	-0.349641000
8	-0.742974000	0.618847000	1.392187000
6	0.781167000	1.616726000	-0.968064000
1	0.980440000	2.258360000	-1.828638000
1	0.790428000	2.254855000	-0.084399000
6	1.874730000	0.547219000	-0.937343000
1	2.100949000	0.223630000	-1.954142000
1	2.792213000	0.925888000	-0.480467000
6	0.588499000	0.536621000	1.846673000
1	1.104336000	1.485995000	1.697584000
1	0.533165000	0.378151000	2.926107000
6	1.428857000	-0.611897000	1.304972000
1	1.084278000	-1.577146000	1.672339000
1	2.450546000	-0.462278000	1.662947000
6	-0.903246000	-1.818402000	-0.160657000
1	-0.780849000	-2.014891000	0.907702000
1	-1.323105000	-2.720921000	-0.607787000
6	0.440037000	-1.623495000	-0.861725000
1	0.906569000	-2.609511000	-0.905454000
1	0.295464000	-1.246823000	-1.871504000
7	1.519144000	-0.731820000	-0.199300000
1	2.363965000	-1.288891000	-0.333595000

4

Sum of electronic and zero-point Energies=	-1826.292604
Sum of electronic and thermal Energies=	-1826.281099
Sum of electronic and thermal Enthalpies=	-1826.280155
Sum of electronic and thermal Free Energies=	-1826.329768

15	0.242983000	-1.666646000	-0.167578000
16	-1.640953000	-1.153359000	-1.031482000
16	1.897828000	-0.645551000	-1.098925000
16	0.252307000	-1.024859000	1.879306000
6	-2.198161000	0.598612000	-0.945865000
1	-2.875785000	0.680245000	-1.798188000
1	-2.791615000	0.746029000	-0.044162000
6	-1.105804000	1.646832000	-1.073646000
1	-0.623766000	1.527213000	-2.045490000
1	-1.590753000	2.640366000	-1.051285000
6	-0.950545000	0.338998000	1.989486000
1	-1.900464000	-0.034785000	1.612207000
1	-1.069862000	0.501171000	3.063686000
6	-0.512210000	1.648326000	1.321373000
1	0.324500000	2.053145000	1.897036000
1	-1.341051000	2.370821000	1.407567000
6	2.257137000	0.856788000	-0.134149000
1	2.294804000	0.587061000	0.923519000
1	3.258772000	1.158407000	-0.448516000
6	1.241188000	1.961283000	-0.383513000

1	1.519388000	2.852885000	0.198092000
1	1.273076000	2.242080000	-1.438027000
7	-0.094077000	1.507186000	-0.055323000

4-H⁺ (P protonated)

Sum of electronic and zero-point Energies=	-1826.648328
Sum of electronic and thermal Energies=	-1826.637311
Sum of electronic and thermal Enthalpies=	-1826.636367
Sum of electronic and thermal Free Energies=	-1826.684852

15	-0.098504000	-0.362011000	-1.062618000
16	1.010731000	-2.021742000	-0.408569000
16	-2.182118000	-0.326674000	-0.915310000
16	1.000959000	1.373375000	-1.462615000
6	2.004806000	-1.101804000	0.807695000
1	2.621730000	-1.842903000	1.315694000
1	2.663287000	-0.418727000	0.270563000
6	1.094284000	-0.398406000	1.813023000
1	0.709395000	-1.134919000	2.517793000
1	1.666461000	0.337562000	2.383937000
6	1.214153000	2.116728000	0.191451000
1	2.183758000	1.827527000	0.595712000
1	1.215727000	3.194624000	0.031730000
6	0.066367000	1.725899000	1.107927000
1	-0.860005000	2.143426000	0.712929000
1	0.228685000	2.128224000	2.113821000
6	-2.502780000	0.179305000	0.805116000
1	-2.735994000	1.242439000	0.826792000
1	-3.391688000	-0.369175000	1.115975000
6	-1.338415000	-0.204535000	1.699692000
1	-1.489338000	0.198987000	2.707656000
1	-1.282964000	-1.292559000	1.764080000
7	-0.054096000	0.262015000	1.149179000
1	-0.176445000	-0.720922000	-2.427184000

4-H⁺ (N_{eq} protonated)

Sum of electronic and zero-point Energies=	-1826.617767
Sum of electronic and thermal Energies=	-1826.605603
Sum of electronic and thermal Enthalpies=	-1826.604659
Sum of electronic and thermal Free Energies=	-1826.656005

15	-0.199650000	-1.726514000	-0.016376000
16	-1.624249000	-0.931353000	-1.295978000
16	2.050083000	-0.952389000	-0.807016000
16	-0.219949000	-0.985328000	1.921943000
6	-2.027080000	0.855140000	-1.130009000
1	-2.631318000	1.028756000	-2.023153000
1	-2.670554000	1.012190000	-0.269131000

6	-0.807178000	1.763760000	-1.147889000
1	-0.303398000	1.645283000	-2.108898000
1	-1.162456000	2.804169000	-1.084155000
6	-1.094272000	0.614312000	1.940617000
1	-2.092418000	0.451263000	1.543725000
1	-1.202633000	0.832106000	3.005442000
6	-0.320814000	1.745741000	1.258517000
1	0.551918000	1.969985000	1.875687000
1	-0.956408000	2.643359000	1.264979000
6	2.436360000	0.604462000	0.063603000
1	2.330915000	0.357935000	1.124006000
1	3.485783000	0.823265000	-0.136905000
6	1.522612000	1.752385000	-0.350143000
1	1.851356000	2.655559000	0.180189000
1	1.659329000	1.952307000	-1.415226000
7	0.129750000	1.434502000	-0.090218000
1	1.674459000	-0.429658000	-1.990753000

4-H⁺ (Nax protonated)

Sum of electronic and zero-point Energies=	-1826.619387
Sum of electronic and thermal Energies=	-1826.607946
Sum of electronic and thermal Enthalpies=	-1826.607002
Sum of electronic and thermal Free Energies=	-1826.656090

15	-1.473286000	-1.046843000	-0.152373000
16	-1.942178000	0.906938000	-0.850771000
16	0.263847000	-1.788356000	-1.224769000
16	-0.766212000	-0.819780000	1.852816000
6	-0.529860000	2.085072000	-0.914828000
1	-0.798998000	2.704303000	-1.772947000
1	-0.522397000	2.747542000	-0.049662000
6	0.838660000	1.522346000	-1.226755000
1	0.757445000	0.672412000	-1.899123000
1	1.429674000	2.294977000	-1.721303000
6	-0.144843000	0.880604000	1.908314000
1	-0.912819000	1.537504000	1.511827000
1	-0.094275000	1.093843000	2.980555000
6	1.258866000	1.221116000	1.416586000
1	1.995939000	0.645303000	1.978930000
1	1.418308000	2.277315000	1.647160000
6	1.701353000	-1.504090000	-0.151699000
1	1.417912000	-1.651212000	0.891426000
1	2.393905000	-2.308877000	-0.409647000
6	2.462483000	-0.212305000	-0.346645000
1	3.333536000	-0.206666000	0.313715000
1	2.811823000	-0.107859000	-1.375431000
7	1.713027000	1.073080000	-0.042163000
1	2.470784000	1.755211000	-0.061029000