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

Supplementary Information

Table of Contents:

(1) Computational details

(2) B3LYP/cc-pVDZ results

Abstract: Cartesian coordinates of two tautomers M^0 and M* and the double proton transfer Transition State structure between them.

- **(I)** 7-Azaindole-Water
- **(II)** 2-amino pyridine -Water
- **(III)** 2-amino pyrazine -Water
- **(IV)** Creatinine -Water
- **(V)** 2-pyrrolyl pyridine -Water
- **(VI)** Quinoline -Water
- **(VII)** Formamide-Water
- **(VIII)** 2-hydroxypyridine -Water
- **(IX)** Piperidine-2-one -Water
- **(X)** Isoxazoline -Water
- **(XI)** Cytosine -Water

(3) MP2/cc-pVDZ results

Abstract: Cartesian coordinates of two tautomers M^0 and M* and the double proton transfer Transition State structure between them.

- **(I)** 7-Azaindole-Water
- **(II)** 2-amino pyridine -Water
- **(III)** 2-amino pyrazine -Water
- **(IV)** Creatinine -Water
- **(V)** 2-pyrrolyl pyridine -Water
- **(VI)** Quinoline -Water
- **(VII)** Formamide-Water
- **(VIII)** 2-hydroxypyridine -Water
- **(IX)** Piperidine-2-one -Water
- **(X)** Isoxazoline -Water
- **(XI)** Cytosine –Water

(4) Calculations for figure 3. Calculation of the BSSE correction.

(5) Table T1. Dipole moments μ^0 (in D) and μ^1 (in D) of M^0 and M^1 tautomers and H-bonding energy.

(6) Table T2. Calculated NICS(1)zz indexes (B3LYP/cc-pVDZ level of theory at points 1 Å above the centers of the aromatic rings) for compounds II,III,VIII,X and XI and their water complexes in both tautomeric forms M^0 and M^1.

(7) Table T3. The relative energy of monomers in ground state S_0 $E_{rel}(M)$(in kcal/mol) and in excited state S^1 $E_{rel}(M^*)$(in kcal/mol); the relative energy of water complexes $M{\bullet}H_2O$ in ground state S_0 $E_{rel}(M{\bullet}H_2O)$ (in kcal/mol) and in excited state S^1 $E_{rel}(M{\bullet}H_2O)^*$ (in kcal/mol); HB stabilization energy of water complexes $M{\bullet}H_2O$ in ground state S_0 $E_{HB}(M{\bullet}H_2O)$ (in kcal/mol) and in excited state S^1 $E_{HB}(M{\bullet}H_2O)^*$ (in kcal/mol).

(1) Computational details:

MP2/cc-pVDZ and DFT B3LYP/cc-pVDZ has been used to investigate the ground state Hydrogen bonded complexes and TS structures of Double proton transfer reactions, using Gaussian[i].

(2) B3LYP/cc-pVDZ results

Abstract: Cartesian coordinates

(Ia) Azaindole-Water ($M^0 \bullet H_2O$) 1^1A - 456.33146.u.; μ=1.6D

C	2.236463000000	0.067680000000	0.036435000000
C	1.041269000000	0.801476000000	0.016299000000
C	-0.169080000000	0.043510000000	-0.022497000000
C	0.884971000000	-1.951714000000	-0.026524000000
C	2.144872000000	-1.324107000000	0.014669000000
C	0.652451000000	2.184297000000	0.021127000000
C	-0.724774000000	2.206994000000	-0.015181000000
N	-0.280219000000	-1.290790000000	-0.045478000000
N	-1.222192000000	0.920687000000	-0.040707000000
H	3.208797000000	0.565553000000	0.066366000000
H	0.817328000000	-3.043325000000	-0.046022000000
H	3.045055000000	-1.941166000000	0.027726000000
H	1.305187000000	3.052947000000	0.046143000000
H	-1.401934000000	3.057703000000	-0.025512000000
H	-2.190523000000	0.586074000000	-0.067678000000
O	-3.133460000000	-1.124510000000	-0.036266000000
H	-3.362011000000	-1.342860000000	0.880597000000
H	-2.234383000000	-1.516937000000	-0.134157000000

(Ib) Azaindole-Water ($M^1 \bullet H_2O$) 1^1A - 456.31798 a.u. ; μ=2.7D

C	-2.206942000000	-0.000002000000	0.026483000000
C	-1.067878000000	0.800779000000	0.013410000000
C	0.225508000000	0.141419000000	-0.013492000000
C	-0.800687000000	-1.983790000000	-0.018221000000
C	-2.062299000000	-1.402211000000	0.010274000000
C	-0.734275000000	2.187924000000	0.014805000000
C	0.655432000000	2.230311000000	-0.012367000000
N	0.311467000000	-1.214313000000	-0.029531000000
N	1.258849000000	0.985966000000	-0.028763000000
H	-3.207141000000	0.440566000000	0.046693000000
H	-0.642785000000	-3.061535000000	-0.033981000000
H	-2.938242000000	-2.050981000000	0.018219000000
H	-1.417307000000	3.033644000000	0.031953000000
H	1.281013000000	3.123835000000	-0.021533000000
H	1.279548000000	-1.590556000000	-0.046223000000
O	3.055941000000	-1.105648000000	-0.052856000000
H	2.719172000000	-0.173521000000	-0.130319000000
H	3.432846000000	-1.124418000000	0.840751000000

$M^0 \bullet H_2O \rightarrow M^1 \bullet H_2O$ TS 1^1A - 456.30009

RC mode i1492

C	2.118684000000	0.514271000000	0.021767000000
C	0.809878000000	1.010247000000	0.012017000000
C	-0.238576000000	0.032678000000	-0.007680000000
C	1.216889000000	-1.752369000000	-0.016495000000
C	2.310069000000	-0.875952000000	0.007736000000
C	0.121634000000	2.265864000000	0.011130000000
C	-1.233095000000	1.959144000000	-0.011266000000
N	-0.049664000000	-1.303017000000	-0.024239000000
N	-1.466932000000	0.600062000000	-0.021480000000
H	2.981891000000	1.184731000000	0.037154000000
H	1.351435000000	-2.835483000000	-0.031771000000
H	3.317580000000	-1.294151000000	0.013139000000
H	0.558591000000	3.261403000000	0.023599000000
H	-2.071415000000	2.654882000000	-0.020793000000
H	-1.246713000000	-1.776240000000	-0.047848000000
O	-2.475255000000	-1.614945000000	-0.064910000000
H	-2.304624000000	-0.442223000000	-0.059834000000
H	-2.801431000000	-1.835982000000	0.822419000000

(IIa) 2-amino pyridine -Water($M^0 \bullet H_2O$) 1^1A -380.11263a.u. ; μ=2.2D

C	0.122011000000	0.686667000000	0.030858000000
C	-1.179961000000	1.243691000000	-0.020908000000
C	-2.272296000000	0.391229000000	-0.042446000000
C	-0.757546000000	-1.453083000000	0.034469000000
C	-2.070875000000	-0.997443000000	-0.010864000000
H	-1.309059000000	2.328156000000	-0.038397000000
H	-3.283533000000	0.803769000000	-0.083116000000
H	-0.543249000000	-2.526808000000	0.052665000000
H	-2.905161000000	-1.699369000000	-0.025889000000
N	0.318486000000	-0.651296000000	0.052537000000
H	2.198068000000	-0.971926000000	-0.136255000000
N	1.242074000000	1.473046000000	0.102763000000
H	1.163893000000	2.430151000000	-0.216352000000
O	3.144212000000	-0.689388000000	-0.159183000000
H	2.129849000000	0.990958000000	-0.073527000000
H	3.423580000000	-0.818452000000	0.760584000000

(IIb) 2-amino pyridine -Water($M^1 \bullet H_2O$) 1^1A 380.09701 a.u. μ=2.4D

C	0.207639000000	0.754101000000	-0.010266000000
C	-1.144104000000	1.282184000000	0.017339000000
C	-2.231076000000	0.451808000000	0.025656000000
C	-0.802252000000	-1.464354000000	-0.018271000000
C	-2.077803000000	-0.968591000000	0.007163000000
H	-1.262391000000	2.367370000000	0.029679000000
H	-3.236014000000	0.881876000000	0.045538000000
H	-0.579169000000	-2.532562000000	-0.035742000000
H	-2.935495000000	-1.638791000000	0.011277000000
N	0.277495000000	-0.642784000000	-0.024100000000
H	1.243555000000	-1.016078000000	-0.042843000000
N	1.337366000000	1.404629000000	-0.025636000000

H	1.173432000000	2.412758000000	-0.020971000000
O	3.060401000000	-0.703109000000	-0.061658000000
H	2.696847000000	0.225916000000	-0.122328000000
H	3.397576000000	-0.739419000000	0.847084000000

IIa →IIb TS 1^1A -378.95195a.u.
RC mode i1482

C	0.255892000000	0.700901000000	-0.008850000000
C	-1.040788000000	1.309715000000	0.015954000000
C	-2.168034000000	0.518739000000	0.023803000000
C	-0.797848000000	-1.438233000000	-0.018657000000
C	-2.065690000000	-0.893814000000	0.006783000000
H	-1.112147000000	2.398876000000	0.027923000000
H	-3.154482000000	0.989535000000	0.042654000000
H	-0.629442000000	-2.517992000000	-0.036249000000
H	-2.947469000000	-1.533174000000	0.010980000000
N	0.312453000000	-0.677733000000	-0.025350000000
H	1.473393000000	-0.996592000000	-0.042627000000
N	1.435388000000	1.313328000000	-0.021437000000
H	1.408358000000	2.327655000000	-0.027171000000
O	2.770758000000	-0.731711000000	-0.066748000000
H	2.348518000000	0.444019000000	-0.056505000000
H	3.111131000000	-0.891656000000	0.828288000000

(IIIa) 2-amino pyrazine -Water($M^0 \bullet H_2O$) 1^1A - -396.14563a.u. μ=1.2D

H	-2.126085000000	0.977646000000	-0.064931000000
C	-0.119043000000	0.658224000000	0.029380000000
C	1.196382000000	1.199114000000	-0.021833000000
C	0.809828000000	-1.437254000000	0.031001000000
C	2.089062000000	-0.895228000000	-0.011751000000
H	1.341211000000	2.285656000000	-0.045277000000
H	0.657679000000	-2.521228000000	0.046353000000
H	2.977846000000	-1.531031000000	-0.026168000000
N	-0.297517000000	-0.679260000000	0.049169000000
O	-3.146482000000	-0.675362000000	-0.152887000000
H	-3.449023000000	-0.834743000000	0.754693000000
H	-2.217568000000	-1.002711000000	-0.133394000000
N	2.279527000000	0.439071000000	-0.042702000000
N	-1.228796000000	1.449200000000	0.095924000000
H	-1.142076000000	2.417105000000	-0.185690000000

(IIIb) 2-amino pyrazine -Water($M^1 \bullet H_2O$) 1^1A -396.12869a.u. μ=1.6D

H	-2.700829000000	0.230641000000	-0.121519000000
C	-0.201654000000	0.733004000000	-0.009391000000
C	1.175657000000	1.229731000000	0.017884000000
C	0.827730000000	-1.446750000000	-0.016854000000
C	2.074259000000	-0.885970000000	0.007545000000
H	1.313496000000	2.318193000000	0.031671000000
H	0.655473000000	-2.524055000000	-0.033007000000
H	2.975563000000	-1.498916000000	0.012342000000

N	-0.277357000000	-0.656742000000	-0.022567000000
O	-3.040870000000	-0.703982000000	-0.064204000000
H	-3.413380000000	-0.745026000000	0.830358000000
H	-1.242150000000	-1.037626000000	-0.039429000000
N	2.239660000000	0.480382000000	0.026008000000
N	-1.306169000000	1.417465000000	-0.023932000000
H	-1.110111000000	2.420813000000	-0.018445000000

IIIa →IIIb TS 1^1A -396.11381a.u.
RC mode i1544

H	-2.352903000000	0.420366000000	-0.056963000000
C	-0.251795000000	0.678374000000	-0.009159000000
C	1.067844000000	1.263025000000	0.016556000000
C	0.832463000000	-1.417860000000	-0.018029000000
C	2.066056000000	-0.801477000000	0.008196000000
H	1.158905000000	2.355519000000	0.030137000000
H	0.721366000000	-2.504875000000	-0.035005000000
H	2.992277000000	-1.378321000000	0.014181000000
N	-0.304302000000	-0.695927000000	-0.025962000000
O	-2.751761000000	-0.730094000000	-0.067655000000
H	-3.107474000000	-0.894925000000	0.820470000000
H	-1.491245000000	-1.013907000000	-0.042656000000
N	2.173080000000	0.556150000000	0.025293000000
N	-1.415904000000	1.311070000000	-0.020850000000
H	-1.364370000000	2.325465000000	-0.023680000000

(IVa) Creatinine -Water($M^0 \bullet H_2O$) 1^1A -469.18164a.u.; μ=3.2D

C	0.321109000000	0.537517000000	-0.068034000000
C	-1.790117000000	-0.140280000000	0.037999000000
N	0.423195000000	-0.758925000000	-0.149337000000
O	-2.987450000000	-0.094302000000	0.124078000000
N	-0.911426000000	-1.169479000000	-0.086630000000
H	-1.162467000000	-2.143230000000	-0.180778000000
O	-0.946189000000	1.002791000000	0.057998000000
N	1.335962000000	1.433713000000	-0.158313000000
H	1.182032000000	2.316303000000	0.317618000000
H	2.258918000000	0.994728000000	-0.044145000000
H	2.426599000000	-1.109276000000	-0.136801000000
O	3.276444000000	-0.666442000000	0.067061000000
H	3.432411000000	-0.915486000000	0.991186000000

(IVb) Creatinine -Water($M^1 \bullet H_2O$) 1^1A - 469.16753a.u. ; μ=2.8D

C	0.363793000000	0.688015000000	0.179910000000
C	-1.713585000000	-0.138212000000	-0.101095000000
N	0.417421000000	-0.670453000000	0.467234000000
O	-2.902077000000	-0.154716000000	-0.230748000000
N	-0.826041000000	-1.198499000000	0.025952000000
H	-1.176891000000	-1.965226000000	0.598125000000
O	-0.946367000000	1.028249000000	-0.064877000000
N	1.373766000000	1.459787000000	0.132526000000

H	1.097710000000	2.416060000000	-0.101290000000
H	2.808045000000	0.190781000000	-0.290345000000
H	1.264618000000	-1.102868000000	0.053713000000
O	3.064690000000	-0.755373000000	-0.391850000000
H	3.619275000000	-0.918689000000	0.386715000000

IVa →IVb TS 1^1A - 469.14586 a.u.
RC mode i1516

C	0.414578000000	0.592254000000	0.137307000000
C	-1.701587000000	-0.090002000000	-0.058960000000
N	0.456272000000	-0.742592000000	0.281532000000
O	-2.896851000000	-0.030242000000	-0.119041000000
N	-0.851959000000	-1.172743000000	-0.026714000000
H	-1.177742000000	-2.015931000000	0.436516000000
O	-0.859497000000	1.042919000000	-0.032563000000
N	1.494776000000	1.327453000000	0.093227000000
H	1.335959000000	2.313460000000	-0.095160000000
H	2.461445000000	0.389616000000	-0.145725000000
H	1.660058000000	-1.055855000000	-0.089253000000
O	2.813126000000	-0.711784000000	-0.290290000000
H	3.294486000000	-0.936770000000	0.522368000000

(Va) 2-pyrrolyl pyridine -Water($M^0 \bullet H_2O$) 1^1A - 533.74908a.u.; μ=2.5D

C	-3.086035000000	-1.243489000000	0.006352000000
C	-3.071325000000	0.146335000000	-0.037743000000
C	-1.737555000000	-1.667170000000	0.028336000000
C	-0.930489000000	-0.522833000000	-0.002541000000
N	-1.776803000000	0.567372000000	-0.042691000000
H	-1.388046000000	-2.696028000000	0.060963000000
H	-1.473841000000	1.552234000000	-0.063498000000
C	0.522612000000	-0.406395000000	-0.003577000000
C	1.337995000000	-1.561136000000	0.033726000000
C	2.718946000000	-1.429711000000	0.028541000000
C	2.417601000000	0.937581000000	-0.047691000000
C	3.286032000000	-0.149244000000	-0.013708000000
H	0.878214000000	-2.548746000000	0.065311000000
H	3.353814000000	-2.318462000000	0.056370000000
H	2.808998000000	1.959568000000	-0.082750000000
H	4.366296000000	0.001264000000	-0.020889000000
N	1.080257000000	0.829539000000	-0.042172000000
H	-3.889676000000	0.861114000000	-0.067618000000
H	-3.971092000000	-1.874709000000	0.019142000000
O	-0.529571000000	3.111465000000	-0.018708000000
H	-0.493332000000	3.355171000000	0.919493000000
H	0.174353000000	2.414869000000	-0.092995000000

(Vb) 2-pyrrolyl pyridine -Water($M^1 \bullet H_2O$) 1^1A - 533.72957a.u. ; μ=4.4D

C	-3.078832000000	-1.237655000000	0.011042000000
C	-3.023657000000	0.182984000000	-0.048716000000

C	-1.759201000000	-1.668608000000	0.041052000000
C	-0.955050000000	-0.487688000000	0.000506000000
N	-1.766968000000	0.638115000000	-0.054201000000
H	-1.411004000000	-2.698858000000	0.089119000000
H	-1.183652000000	2.216795000000	-0.112633000000
C	0.459693000000	-0.411827000000	0.004188000000
C	1.314765000000	-1.557176000000	0.019983000000
C	2.682725000000	-1.422545000000	0.009626000000
C	2.444992000000	0.951733000000	-0.027209000000
C	3.282616000000	-0.135325000000	-0.017584000000
H	0.855795000000	-2.544163000000	0.034792000000
H	3.313335000000	-2.314399000000	0.019272000000
H	2.800958000000	1.982755000000	-0.047686000000
H	4.363352000000	-0.003329000000	-0.031236000000
N	1.097227000000	0.808146000000	-0.011914000000
H	-3.866314000000	0.875551000000	-0.090357000000
H	-3.976269000000	-1.853674000000	0.028200000000
O	-0.531042000000	2.991885000000	-0.031294000000
H	-0.687162000000	3.308268000000	0.872430000000
H	0.519168000000	1.688786000000	-0.006078000000

Va →Vb TS 1^1A - 533.72460 a.u.
RC mode i1207

C	-3.097748000000	-1.174102000000	0.007608000000
C	-3.043230000000	0.233570000000	-0.048890000000
C	-1.771432000000	-1.616317000000	0.039063000000
C	-0.955681000000	-0.457773000000	0.002303000000
N	-1.768546000000	0.663180000000	-0.052285000000
H	-1.434351000000	-2.649985000000	0.083498000000
H	-1.251100000000	1.863999000000	-0.063988000000
C	0.476680000000	-0.381384000000	0.002853000000
C	1.306397000000	-1.536971000000	0.023287000000
C	2.680965000000	-1.415211000000	0.013221000000
C	2.442438000000	0.957304000000	-0.034059000000
C	3.281895000000	-0.137784000000	-0.018105000000
H	0.838739000000	-2.520202000000	0.042583000000
H	3.304331000000	-2.312233000000	0.027206000000
H	2.817488000000	1.983088000000	-0.059262000000
H	4.363726000000	-0.009842000000	-0.030686000000
N	1.099880000000	0.837215000000	-0.020682000000
H	-3.869195000000	0.943329000000	-0.088992000000
H	-3.996682000000	-1.786986000000	0.021780000000
O	-0.486019000000	2.776676000000	-0.025955000000
H	-0.565324000000	3.123516000000	0.876799000000
H	0.439471000000	1.821159000000	-0.014222000000

(VIa) Quinoline -Water(M^0•H_2O) 1^1A - 609.98940a.u.; μ=1.9D

C	-2.998062000000	-0.879129000000	-0.008559000000
C	-3.067097000000	0.500593000000	-0.040640000000
C	-1.608936000000	-1.219234000000	0.007206000000
C	-0.890877000000	0.003184000000	-0.015851000000
N	-1.800270000000	1.029745000000	-0.045103000000

H	-1.540480000000	2.028677000000	-0.056196000000
C	0.532685000000	0.049298000000	-0.015156000000
C	1.217263000000	-1.214241000000	0.014003000000
C	2.629722000000	-1.175782000000	0.012887000000
C	2.526438000000	1.221150000000	-0.044923000000
C	3.291959000000	0.038705000000	-0.016868000000
H	3.188637000000	-2.115349000000	0.034578000000
H	3.022719000000	2.196779000000	-0.071046000000
H	4.381683000000	0.093766000000	-0.019972000000
N	1.199146000000	1.239929000000	-0.043142000000
H	-3.935672000000	1.154365000000	-0.062206000000
H	-3.841924000000	-1.564218000000	0.000495000000
C	0.477046000000	-2.442644000000	0.040445000000
H	1.036976000000	-3.380614000000	0.062256000000
C	-0.896656000000	-2.451758000000	0.036676000000
H	-1.443642000000	-3.397360000000	0.055229000000
O	-0.472823000000	3.492160000000	0.001387000000
H	-0.409454000000	3.762397000000	0.930722000000
H	0.250702000000	2.815720000000	-0.082562000000

(VIb) Quinoline -Water(M^1•H_2O) 1^1A - 609.96961a.u.; μ=4.2D

C	-3.025116000000	-0.795702000000	-0.008056000000
C	-3.019861000000	0.610227000000	-0.041545000000
C	-1.667256000000	-1.177130000000	0.009452000000
C	-0.929256000000	0.059979000000	-0.012320000000
N	-1.771823000000	1.139440000000	-0.044078000000
H	-1.063551000000	2.660992000000	-0.090048000000
C	0.477479000000	0.034146000000	-0.008602000000
C	1.165230000000	-1.240440000000	0.011388000000
C	2.566598000000	-1.222035000000	0.004770000000
C	2.578110000000	1.174146000000	-0.033605000000
C	3.284701000000	-0.020767000000	-0.020150000000
H	3.104553000000	-2.173603000000	0.018341000000
H	3.059274000000	2.152571000000	-0.051222000000
H	4.373965000000	-0.008335000000	-0.028241000000
N	1.235890000000	1.178872000000	-0.025328000000
H	-3.890313000000	1.267984000000	-0.066256000000
H	-3.897454000000	-1.446131000000	-0.000950000000
C	0.397674000000	-2.451395000000	0.034739000000
H	0.936686000000	-3.400857000000	0.050650000000
C	-0.977521000000	-2.421122000000	0.034935000000
H	-1.542377000000	-3.357128000000	0.051871000000
O	-0.336799000000	3.370404000000	-0.011838000000
H	-0.460771000000	3.707578000000	0.889335000000
H	0.721213000000	2.106078000000	-0.018967000000

VIa →VIb TS 1^1A - 609.96473a.u.
RC mode i1238

C	-3.029153000000	-0.752138000000	-0.010483000000
C	-3.025290000000	0.644375000000	-0.042898000000
C	-1.665605000000	-1.145200000000	0.008423000000
C	-0.917166000000	0.072991000000	-0.011599000000

N	-1.760198000000	1.150664000000	-0.044363000000
H	-1.175097000000	2.333248000000	-0.046350000000
C	0.497732000000	0.054490000000	-0.009507000000
C	1.168168000000	-1.221621000000	0.012289000000
C	2.574950000000	-1.206904000000	0.006602000000
C	2.565240000000	1.191506000000	-0.038709000000
C	3.282647000000	-0.007300000000	-0.020576000000
H	3.113409000000	-2.158317000000	0.022377000000
H	3.059639000000	2.165163000000	-0.060188000000
H	4.372465000000	0.010452000000	-0.028032000000
N	1.231131000000	1.210591000000	-0.031560000000
H	-3.883301000000	1.315870000000	-0.067498000000
H	-3.903884000000	-1.398708000000	-0.004704000000
C	0.393443000000	-2.428245000000	0.036021000000
H	0.926006000000	-3.381567000000	0.053237000000
C	-0.982073000000	-2.393486000000	0.034362000000
H	-1.551433000000	-3.326456000000	0.050375000000
O	-0.330922000000	3.163798000000	-0.005967000000
H	-0.377447000000	3.519240000000	0.895772000000
H	0.593128000000	2.231094000000	-0.019342000000

(VIIa) Formamide (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A - 246.34610a.u. ; μ=2.2D

C	-1.190533000000	-0.166067000000	0.015657000000
N	-0.682145000000	1.083121000000	0.005452000000
H	0.340712000000	1.172806000000	-0.042980000000
H	-2.304059000000	-0.198654000000	0.050387000000
H	-1.289410000000	1.891525000000	-0.010076000000
O	-0.518109000000	-1.194510000000	-0.005972000000
O	1.962968000000	0.092985000000	-0.092168000000
H	2.333990000000	-0.025928000000	0.795750000000
H	1.278103000000	-0.612996000000	-0.140070000000

(VIIb) Formamide (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -246.33156a.u. ; μ=3.2D

C	1.177762000000	-0.062814000000	0.018321000000
N	0.644060000000	1.102234000000	-0.006090000000
H	-0.496878000000	-0.932118000000	-0.048579000000
H	2.260842000000	-0.266045000000	0.059234000000
H	1.358354000000	1.833177000000	0.011160000000
O	0.473123000000	-1.187429000000	-0.003354000000
O	-1.880397000000	0.073370000000	-0.092656000000
H	-2.248923000000	0.152883000000	0.801203000000
H	-1.190198000000	0.785824000000	-0.122233000000

(VIIa)-(VIIb) TS 1^1A - 246.31735a.u.
RC mode i1523

C	1.089924000000	-0.116083000000	0.017297000000
N	0.554751000000	1.080039000000	-0.000876000000
H	-0.750335000000	0.869041000000	-0.059578000000
H	2.186849000000	-0.251543000000	0.050260000000

H	1.208531000000	1.858262000000	0.003055000000
O	0.377568000000	-1.182971000000	-0.002986000000
O	-1.656122000000	0.095293000000	-0.098897000000
H	-2.066451000000	0.105169000000	0.780765000000
H	-0.772967000000	-0.743279000000	-0.057095000000

(VIIIa) 2-hydroxyl-pyridine (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A - 399.98744a.u.; μ=2.4D

H	2.067058000000	0.803516000000	-0.065068000000
O	1.267965000000	1.400748000000	-0.034052000000
N	0.302874000000	-0.697034000000	-0.038555000000
C	-2.227194000000	0.483467000000	0.035255000000
C	-1.089817000000	1.275534000000	0.020239000000
C	0.169410000000	0.640148000000	-0.017181000000
C	-0.815525000000	-1.445674000000	-0.025033000000
C	-2.098724000000	-0.914901000000	0.012117000000
H	-3.215841000000	0.948057000000	0.063660000000
H	-0.659389000000	-2.528813000000	-0.045581000000
H	-2.970599000000	-1.569906000000	0.021515000000
H	-1.133529000000	2.364901000000	0.035008000000
O	3.063922000000	-0.599047000000	-0.048544000000
H	2.173721000000	-1.027923000000	-0.101234000000
H	3.334457000000	-0.755644000000	0.869965000000

(VIIIb) 2-hydroxyl-pyridine (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -399.98876a.u. ; μ=3.4D

H	2.676206000000	0.264357000000	-0.128982000000
O	1.272175000000	1.418882000000	-0.029338000000
N	0.278509000000	-0.646926000000	-0.025984000000
C	-2.216039000000	0.469814000000	0.027849000000
C	-1.119264000000	1.292516000000	0.018307000000
C	0.222926000000	0.752788000000	-0.012307000000
C	-0.807503000000	-1.463838000000	-0.018373000000
C	-2.075860000000	-0.948114000000	0.008527000000
H	-3.217891000000	0.907233000000	0.049186000000
H	-0.598622000000	-2.534974000000	-0.035566000000
H	-2.941433000000	-1.608715000000	0.013727000000
H	-1.206172000000	2.379291000000	0.030621000000
O	3.057863000000	-0.646344000000	-0.056866000000
H	1.242537000000	-1.023399000000	-0.040168000000
H	3.429950000000	-0.654613000000	0.838680000000

(VIIIa)-(VIIIb) TS 1^1A -398.81696a.u.
RC mode i1515

H	2.263816000000	0.450730000000	-0.059113000000
O	1.389463000000	1.323857000000	-0.025628000000
N	0.318502000000	-0.695240000000	-0.024611000000
C	-2.14564600009900	0.546539000000	0.024703000000

C	-0.999547000000	1.315413000000	0.015602000000
C	0.273094000000	0.675798000000	-0.009872000000
C	-0.808106000000	-1.435784000000	-0.017786000000
C	-2.065155000000	-0.864132000000	0.007484000000
H	-3.123925000000	1.033937000000	0.043498000000
H	-0.666135000000	-2.519598000000	-0.034338000000
H	-2.958517000000	-1.488118000000	0.012058000000
H	-1.025188000000	2.405215000000	0.025713000000
O	2.746158000000	-0.655810000000	-0.064648000000
H	1.562478000000	-0.994108000000	-0.040762000000
H	3.105148000000	-0.792755000000	0.826644000000

(IXa) piperidine-2-one (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -402.40735a.u. ; μ=3.8D

C	-2.172019000000	0.489430000000	0.372993000000
C	-1.014123000000	1.388210000000	-0.073620000000
C	0.351494000000	0.714349000000	-0.054614000000
N	0.389507000000	-0.642085000000	-0.051567000000
C	-0.744937000000	-1.549273000000	0.089549000000
C	-2.057706000000	-0.876987000000	-0.306703000000
H	-3.136673000000	0.967573000000	0.139066000000
H	-2.144230000000	0.356291000000	1.469987000000
H	-0.929303000000	2.301841000000	0.533137000000
H	-1.171903000000	1.726586000000	-1.113891000000
H	1.343549000000	-1.025014000000	-0.022466000000
H	-0.559607000000	-2.437716000000	-0.536064000000
H	-0.814468000000	-1.906853000000	1.136209000000
H	-2.897431000000	-1.534541000000	-0.030518000000
H	-2.091481000000	-0.747621000000	-1.403339000000
O	1.386192000000	1.395811000000	-0.085842000000
O	3.253083000000	-0.628491000000	-0.009115000000
H	2.822700000000	0.252839000000	-0.126414000000
H	3.561844000000	-0.591727000000	0.909282000000

(IXb) piperidine-2-ol (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -402.39231; μ=2.6D

C	0.741422000000	-1.534323000000	0.095631000000
C	0.983863000000	1.375289000000	-0.047879000000
C	-0.312440000000	0.598130000000	-0.028546000000
N	-0.444725000000	-0.678932000000	0.034118000000
C	2.183227000000	0.502721000000	0.334510000000
C	2.048714000000	-0.864560000000	-0.338921000000
H	0.543874000000	-2.424685000000	-0.524920000000
H	0.840668000000	-1.909627000000	1.133159000000
H	0.868860000000	2.246490000000	0.616246000000
H	1.101569000000	1.786513000000	-1.066939000000
H	3.124046000000	1.000829000000	0.051822000000
H	2.211596000000	0.369179000000	1.431128000000
H	2.901218000000	-1.518342000000	-0.091374000000
H	2.049957000000	-0.734673000000	-1.436672000000
O	-1.384940000000	1.397856000000	-0.100820000000

H	-2.199509000000	0.818083000000	-0.115690000000
O	-3.174494000000	-0.603163000000	-0.044132000000
H	-2.258865000000	-0.994569000000	-0.040779000000
H	-3.463586000000	-0.707762000000	0.876037000000

(IXa)-(IXb) TS 1^1A -402.37935a.u.
RC mode i1502

C	0.739238000000	-1.527677000000	0.104195000000
C	0.896428000000	1.406465000000	-0.053847000000
C	-0.397761000000	0.625591000000	-0.025266000000
N	-0.450703000000	-0.685070000000	0.039140000000
C	2.113593000000	0.557915000000	0.329378000000
C	2.016035000000	-0.813269000000	-0.344565000000
H	0.559071000000	-2.421126000000	-0.516653000000
H	0.863724000000	-1.894979000000	1.141856000000
H	0.770537000000	2.284851000000	0.597912000000
H	1.000743000000	1.804669000000	-1.079305000000
H	3.043447000000	1.076458000000	0.047041000000
H	2.146028000000	0.424856000000	1.425992000000
H	2.891128000000	-1.439215000000	-0.105492000000
H	2.000735000000	-0.683549000000	-1.441972000000
O	-1.493323000000	1.316425000000	-0.092906000000
H	-2.351665000000	0.503251000000	-0.093341000000
O	-2.883504000000	-0.645950000000	-0.052929000000
H	-1.710868000000	-0.976155000000	0.016058000000
H	-3.248540000000	-0.741519000000	0.841227000000

(Xa) Isoxazoline (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -397.72946a.u. ; μ=1.8D

C	1.467238000000	0.963792000000	0.027191000000
C	2.119306000000	-0.229365000000	0.022069000000
O	1.253388000000	-1.257520000000	-0.011808000000
N	-0.046600000000	-0.741076000000	-0.029251000000
H	-1.777349000000	0.845810000000	-0.055860000000
H	1.874543000000	1.968832000000	0.049528000000
H	3.172020000000	-0.502667000000	0.039421000000
C	0.089594000000	0.576456000000	-0.007634000000
O	-0.950165000000	1.405698000000	-0.020805000000
O	-2.794897000000	-0.543874000000	-0.062763000000
H	-1.986677000000	-1.094867000000	-0.161260000000
H	-3.079774000000	-0.729303000000	0.846178000000

(Xb) Isoxazoline (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -397.72197a.u. ; μ=2.6D

C	-1.490996000000	0.932730000000	-0.106361000000
C	-2.047688000000	-0.297560000000	-0.147682000000
O	-1.154382000000	-1.297665000000	0.039147000000
N	0.057054000000	-0.652440000000	0.314450000000
H	0.905817000000	-1.147796000000	-0.004023000000

H	-1.976655000000	1.892755000000	-0.245736000000
H	-3.070744000000	-0.639435000000	-0.292784000000
C	-0.058829000000	0.720806000000	0.096890000000
O	0.901196000000	1.494138000000	0.098141000000
O	2.720508000000	-0.606446000000	-0.270190000000
H	3.221155000000	-0.705847000000	0.554270000000
H	2.367548000000	0.311323000000	-0.206738000000

(Xa)-(Xb) TS 1^1A - 397.70372a.u.
RC mode i1372

C	1.393772000000	0.998582000000	0.002797000000
C	2.040690000000	-0.193740000000	-0.010188000000
O	1.189323000000	-1.242949000000	-0.001524000000
N	-0.089986000000	-0.700520000000	0.032012000000
H	-2.022010000000	0.424876000000	-0.076594000000
H	1.817830000000	1.996967000000	-0.005256000000
H	3.093976000000	-0.465720000000	-0.025327000000
C	-0.011038000000	0.648434000000	0.017229000000
O	-1.064472000000	1.372612000000	0.003625000000
O	-2.455417000000	-0.623137000000	-0.111855000000
H	-1.309225000000	-1.057494000000	-0.063397000000
H	-2.846681000000	-0.766853000000	0.765499000000

(XIa) Cytosine (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A - 471.40763a.u. ; μ=5.4D

H	2.991621000000	-0.565464000000	-0.129992000000
O	1.441523000000	-1.484377000000	-0.035579000000
N	0.785145000000	0.698455000000	-0.021074000000
C	-1.761116000000	-0.136075000000	0.013689000000
C	0.497162000000	-0.686776000000	-0.016265000000
C	-0.183584000000	1.640374000000	-0.019683000000
C	-1.498845000000	1.278500000000	-0.001792000000
H	0.146311000000	2.681335000000	-0.032124000000
H	-2.295456000000	2.020614000000	0.008456000000
N	-0.815637000000	-1.063748000000	0.001806000000
N	-3.050628000000	-0.575016000000	0.075978000000
H	-3.192774000000	-1.567548000000	-0.074233000000
H	-3.807548000000	0.050186000000	-0.165689000000
O	3.524177000000	0.266651000000	-0.049051000000
H	1.793238000000	0.925980000000	-0.030802000000
H	3.885149000000	0.202738000000	0.848752000000

(XIb) Cytosine (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A - 471.40645a.u. ; μ=4.1D

H	2.298028000000	-1.010767000000	-0.068308000000
O	1.416410000000	-1.476671000000	-0.042143000000
N	0.829336000000	0.743906000000	-0.036607000000
C	-1.776996000000	-0.121103000000	0.018265000000
C	0.457750000000	-0.556809000000	-0.023453000000

C	-0.180681000000	1.632377000000	-0.027033000000
C	-1.513695000000	1.271409000000	0.001427000000
H	0.110127000000	2.687860000000	-0.042843000000
H	-2.310869000000	2.014932000000	0.015099000000
N	-0.791768000000	-1.028692000000	0.000692000000
N	-3.050323000000	-0.611029000000	0.090722000000
H	-3.152854000000	-1.602171000000	-0.097437000000
H	-3.821579000000	-0.012198000000	-0.173580000000
O	3.525013000000	0.199038000000	-0.036631000000
H	2.715613000000	0.766722000000	-0.090361000000
H	3.801160000000	0.292160000000	0.888738000000

(XIa)-(XIb) TS 1^1A - 471.38863 a.u.
RC mode i1526

H	2.520728000000	-0.757869000000	-0.058685000000
O	1.502601000000	-1.446896000000	-0.030788000000
N	0.849792000000	0.730752000000	-0.020374000000
C	-1.718474000000	-0.139281000000	0.013069000000
C	0.526116000000	-0.614322000000	-0.013315000000
C	-0.142938000000	1.637210000000	-0.018627000000
C	-1.465753000000	1.264825000000	-0.001027000000
H	0.158932000000	2.688342000000	-0.031518000000
H	-2.268781000000	2.001093000000	0.007274000000
N	-0.746369000000	-1.054111000000	0.002369000000
N	-2.994816000000	-0.614354000000	0.071594000000
H	-3.110517000000	-1.608358000000	-0.090415000000
H	-3.766957000000	-0.006952000000	-0.167336000000
O	3.222444000000	0.231790000000	-0.058937000000
H	2.119616000000	0.790114000000	-0.033579000000
H	3.592672000000	0.287878000000	0.836346000000

(3) MP2/cc-pVDZ results

Abstract: Cartesian coordinates

(Ia) Azaindole-Water($M^0 \bullet H_2O$) 1^1A -454.98273a.u.

C	2.252546000000	0.083024000000	0.037206000000
C	1.041380000000	0.810187000000	0.016584000000
C	-0.167580000000	0.039618000000	-0.022361000000
C	0.900218000000	-1.954522000000	-0.027113000000
C	2.163086000000	-1.312166000000	0.014880000000
C	0.647378000000	2.188293000000	0.021438000000
C	-0.745118000000	2.199263000000	-0.015703000000
N	-0.278469000000	-1.303806000000	-0.046637000000
N	-1.228796000000	0.911596000000	-0.041820000000
H	3.224006000000	0.588660000000	0.067203000000
H	0.843241000000	-3.048896000000	-0.047220000000
H	3.067762000000	-1.927850000000	0.027924000000
H	1.292543000000	3.066099000000	0.046494000000

H	-1.430394000000	3.047460000000	-0.026074000000
H	-2.197058000000	0.573274000000	-0.066043000000
O	-3.147172000000	-1.123117000000	-0.033805000000
H	-3.364735000000	-1.366530000000	0.876497000000
H	-2.258603000000	-1.523988000000	-0.138729000000

(Ib) Azaindole-Water ($M^1 \bullet H_2O$) 1^1A -454.96740a.u.

C	-2.221156000000	-0.045858000000	0.025047000000
C	-1.084308000000	0.787033000000	0.013109000000
C	0.226150000000	0.155074000000	-0.011029000000
C	-0.751593000000	-2.000314000000	-0.017374000000
C	-2.039844000000	-1.439277000000	0.009243000000
C	-0.787485000000	2.175208000000	0.014107000000
C	0.618379000000	2.248834000000	-0.012023000000
N	0.338224000000	-1.202057000000	-0.027488000000
N	1.253968000000	1.023316000000	-0.027092000000
H	-3.232589000000	0.376128000000	0.043342000000
H	-0.568013000000	-3.076713000000	-0.032895000000
H	-2.898336000000	-2.115800000000	0.015981000000
H	-1.488976000000	3.009832000000	0.029718000000
H	1.219965000000	3.162384000000	-0.021223000000
H	1.315788000000	-1.559137000000	-0.042454000000
O	3.068246000000	-1.076529000000	-0.053850000000
H	2.741477000000	-0.148305000000	-0.137538000000
H	3.458507000000	-1.069174000000	0.831443000000

$M^0 \bullet H_2O \rightarrow M^1 \bullet H_2O$ TS 1^1A -454.95093
RC mode i1277

C	2.142408000000	0.484951000000	0.023032000000
C	0.827933000000	1.004107000000	0.012421000000
C	-0.242150000000	0.039789000000	-0.006844000000
C	1.186813000000	-1.775984000000	-0.017913000000
C	2.303058000000	-0.908211000000	0.007573000000
C	0.167731000000	2.267142000000	0.011213000000
C	-1.208314000000	1.978266000000	-0.012488000000
N	-0.075703000000	-1.306239000000	-0.025808000000
N	-1.470646000000	0.627314000000	-0.022578000000
H	3.018539000000	1.143397000000	0.038851000000
H	1.307036000000	-2.863517000000	-0.034852000000
H	3.303993000000	-1.349838000000	0.012824000000
H	0.619814000000	3.259440000000	0.023625000000
H	-2.033324000000	2.694953000000	-0.022775000000
H	-1.320933000000	-1.753263000000	-0.051870000000
O	-2.500925000000	-1.585306000000	-0.062907000000
H	-2.334052000000	-0.464369000000	-0.068952000000
H	-2.794104000000	-1.772244000000	0.843146000000

(IIa) 2-amino pyridine -Water($M^0 \bullet H_2O$) 1^1A -378.98838a.u.

C	0.113193000000	0.689010000000	0.046377000000
C	-1.190176000000	1.239652000000	-0.037899000000

C	-2.289666000000	0.382743000000	-0.075868000000
C	-0.755651000000	-1.460635000000	0.061733000000
C	-2.075175000000	-1.007138000000	-0.020614000000
H	-1.321042000000	2.326356000000	-0.067644000000
H	-3.303084000000	0.792149000000	-0.144076000000
H	-0.536477000000	-2.534342000000	0.100480000000
H	-2.905648000000	-1.717571000000	-0.045238000000
N	0.322922000000	-0.647145000000	0.092905000000
H	2.239478000000	-0.973133000000	-0.142994000000
N	1.232474000000	1.500228000000	0.158135000000
H	1.145370000000	2.398407000000	-0.308813000000
O	3.176630000000	-0.692428000000	-0.203955000000
H	2.100119000000	1.006166000000	-0.073251000000
H	3.465313000000	-0.791981000000	0.713534000000

(IIb) 2-amino pyridine -Water($M^1 \bullet H_2O$) 1^1A -378.96793a.u.

C	0.206719000000	0.761815000000	-0.008220000000
C	-1.152411000000	1.279756000000	0.015139000000
C	-2.245707000000	0.442180000000	0.022129000000
C	-0.794257000000	-1.469517000000	-0.015369000000
C	-2.080721000000	-0.979612000000	0.006156000000
H	-1.280986000000	2.366951000000	0.025816000000
H	-3.252857000000	0.873194000000	0.038846000000
H	-0.559687000000	-2.537495000000	-0.031045000000
H	-2.931980000000	-1.661829000000	0.009001000000
N	0.280363000000	-0.632642000000	-0.019613000000
H	1.246093000000	-1.004685000000	-0.037301000000
N	1.338122000000	1.423971000000	-0.021228000000
H	1.138086000000	2.428500000000	-0.019281000000
O	3.071250000000	-0.712739000000	-0.065341000000
H	2.724735000000	0.212102000000	-0.135067000000
H	3.415460000000	-0.721863000000	0.838631000000

IIa →IIb TS 1^1A -378.95195a.u.
RC mode i1590

C	0.264772000000	0.700006000000	-0.005490000000
C	-1.034775000000	1.311890000000	0.013033000000
C	-2.175788000000	0.525643000000	0.019337000000
C	-0.800316000000	-1.441351000000	-0.015058000000
C	-2.073555000000	-0.889597000000	0.005450000000
H	-1.104272000000	2.404362000000	0.022471000000
H	-3.160868000000	1.005136000000	0.033689000000
H	-0.634527000000	-2.523817000000	-0.030697000000
H	-2.956621000000	-1.531685000000	0.008227000000
N	0.316301000000	-0.679001000000	-0.019454000000
H	1.511927000000	-0.989484000000	-0.045619000000
N	1.450456000000	1.312846000000	-0.014481000000
H	1.400915000000	2.328394000000	-0.032329000000
O	2.756629000000	-0.736115000000	-0.073479000000
H	2.371602000000	0.394721000000	-0.067704000000
H	3.069476000000	-0.875171000000	0.833719000000

(IIIa) 2-amino pyrazine -Water($M^0 \bullet H_2O$) 1^1A -395.00373a.u.

H	-2.096718000000	0.992067000000	-0.060606000000
C	-0.110881000000	0.660907000000	0.048900000000
C	1.204550000000	1.193441000000	-0.043624000000
C	0.806789000000	-1.445049000000	0.062035000000
C	2.091714000000	-0.904214000000	-0.025701000000
H	1.351490000000	2.280669000000	-0.084835000000
H	0.651592000000	-2.529411000000	0.100024000000
H	2.975276000000	-1.550275000000	-0.053584000000
N	-0.305702000000	-0.677713000000	0.097606000000
O	-3.175575000000	-0.675459000000	-0.204849000000
H	-3.501279000000	-0.811131000000	0.695468000000
H	-2.256474000000	-1.003576000000	-0.134736000000
N	2.303771000000	0.432449000000	-0.084697000000
N	-1.219103000000	1.474910000000	0.159147000000
H	-1.125086000000	2.387300000000	-0.276989000000

(IIIb) 2-amino pyrazine -Water($M^1 \bullet H_2O$) 1^1A -394.98117a.u.

H	-2.726877000000	0.219554000000	-0.133431000000
C	-0.200571000000	0.740207000000	-0.006571000000
C	1.181289000000	1.224295000000	0.014664000000
C	0.817446000000	-1.451928000000	-0.013217000000
C	2.076006000000	-0.894487000000	0.006123000000
H	1.328514000000	2.313502000000	0.025429000000
H	0.636798000000	-2.529911000000	-0.026996000000
H	2.969808000000	-1.521544000000	0.009251000000
N	-0.283112000000	-0.648707000000	-0.016878000000
O	-3.049355000000	-0.712070000000	-0.069091000000
H	-3.435235000000	-0.727556000000	0.817810000000
H	-1.248336000000	-1.027157000000	-0.031997000000
N	2.262725000000	0.471945000000	0.021181000000
N	-1.308185000000	1.437518000000	-0.018143000000
H	-1.074844000000	2.435863000000	-0.016448000000

IIIa →IIIb TS 1^1A -394.96626a.u.
RC mode i1556

H	-2.379200000000	0.374257000000	-0.068698000000
C	-0.259195000000	0.678723000000	-0.004654000000
C	1.062431000000	1.261602000000	0.012544000000
C	0.833261000000	-1.422377000000	-0.013605000000
C	2.072102000000	-0.797008000000	0.006318000000
H	1.152556000000	2.356326000000	0.021346000000
H	0.726146000000	-2.511863000000	-0.028340000000
H	2.997343000000	-1.379515000000	0.010369000000
N	-0.310236000000	-0.699302000000	-0.018353000000
O	-2.744831000000	-0.732421000000	-0.076399000000
H	-3.071880000000	-0.874279000000	0.825623000000

H	-1.528237000000	-1.006278000000	-0.044374000000
N	2.191096000000	0.563119000000	0.019164000000
N	-1.429172000000	1.314179000000	-0.012158000000
H	-1.351488000000	2.329112000000	-0.028926000000

(IVa) Creatinine -Water($M^0 \bullet H_2O$) 1^1A -467.93071a.u.

C	0.313606000000	0.539013000000	-0.075005000000
C	-1.792583000000	-0.140557000000	0.043018000000
N	0.422603000000	-0.761300000000	-0.172038000000
O	-2.994437000000	-0.107202000000	0.141030000000
N	-0.906105000000	-1.168334000000	-0.099770000000
H	-1.157176000000	-2.142742000000	-0.204499000000
O	-0.952993000000	1.003511000000	0.066482000000
N	1.325244000000	1.454162000000	-0.185746000000
H	1.181577000000	2.274734000000	0.398064000000
H	2.237473000000	1.000728000000	-0.053825000000
H	2.470171000000	-1.115206000000	-0.144056000000
O	3.301606000000	-0.664850000000	0.090753000000
H	3.416218000000	-0.931617000000	1.012992000000

(IVb) Creatinine -Water($M^1 \bullet H_2O$) 1^1A -467.91544a.u.

C	0.354252000000	0.697708000000	0.186059000000
C	-1.709473000000	-0.143785000000	-0.106474000000
N	0.412459000000	-0.657917000000	0.515629000000
O	-2.901087000000	-0.174242000000	-0.244697000000
N	-0.809519000000	-1.203094000000	0.023958000000
H	-1.177487000000	-1.942611000000	0.623964000000
O	-0.953743000000	1.031788000000	-0.077627000000
N	1.368832000000	1.475185000000	0.139947000000
H	1.062425000000	2.419432000000	-0.116555000000
H	2.832104000000	0.176371000000	-0.310038000000
H	1.255600000000	-1.079166000000	0.089140000000
O	3.069244000000	-0.767501000000	-0.411945000000
H	3.640977000000	-0.917147000000	0.353391000000

IVa →IVb TS 1^1A -467.89076a.u.
RC mode i1464

C	0.415555000000	0.590339000000	0.147856000000
C	-1.695823000000	-0.085997000000	-0.063031000000
N	0.456197000000	-0.744102000000	0.313779000000
O	-2.896087000000	-0.032283000000	-0.127774000000
N	-0.843087000000	-1.176596000000	-0.028732000000
H	-1.184482000000	-1.987831000000	0.483141000000
O	-0.856624000000	1.046910000000	-0.047541000000
N	1.501125000000	1.328367000000	0.112261000000
H	1.319155000000	2.306906000000	-0.103871000000
H	2.461324000000	0.360323000000	-0.166632000000
H	1.674482000000	-1.039369000000	-0.094425000000

O	2.795988000000	-0.713949000000	-0.314231000000
H	3.265260000000	-0.925189000000	0.508039000000

(Va) 2-pyrrolyl pyridine -Water($M^0 \bullet H_2O$) 1^1A -532.15037a.u.

C	-3.089253000000	-1.259294000000	0.007405000000
C	-3.073257000000	0.140384000000	-0.038302000000
C	-1.738978000000	-1.688588000000	0.030733000000
C	-0.926645000000	-0.534934000000	-0.000976000000
N	-1.769541000000	0.554241000000	-0.043190000000
H	-1.387057000000	-2.719933000000	0.065104000000
H	-1.464145000000	1.538444000000	-0.064032000000
C	0.529755000000	-0.411224000000	-0.003040000000
C	1.350031000000	-1.565544000000	0.029418000000
C	2.740053000000	-1.429703000000	0.024980000000
C	2.417665000000	0.951707000000	-0.043096000000
C	3.295182000000	-0.138718000000	-0.012839000000
H	0.889388000000	-2.556676000000	0.056616000000
H	3.381880000000	-2.316537000000	0.049246000000
H	2.805556000000	1.977228000000	-0.075294000000
H	4.377059000000	0.021168000000	-0.019712000000
N	1.072004000000	0.836791000000	-0.037571000000
H	-3.888697000000	0.862291000000	-0.070046000000
H	-3.979274000000	-1.888511000000	0.020295000000
O	-0.564158000000	3.139664000000	-0.022611000000
H	-0.514243000000	3.380064000000	0.913184000000
H	0.148216000000	2.463406000000	-0.094852000000

(Vb) 2-pyrrolyl pyridine -Water($M^1 \bullet H_2O$) 1^1A -532.12610a.u.

C	-3.101362000000	-1.218710000000	0.016220000000
C	-3.034105000000	0.201555000000	-0.053972000000
C	-1.776365000000	-1.669008000000	0.050839000000
C	-0.967231000000	-0.487119000000	0.001755000000
N	-1.756013000000	0.651358000000	-0.061495000000
H	-1.434863000000	-2.704619000000	0.109846000000
H	-1.145577000000	2.243171000000	-0.132851000000
C	0.455283000000	-0.417742000000	0.005904000000
C	1.305789000000	-1.566272000000	0.009375000000
C	2.686629000000	-1.438202000000	-0.000014000000
C	2.442446000000	0.949031000000	-0.016350000000
C	3.283442000000	-0.150091000000	-0.016980000000
H	0.840284000000	-2.554285000000	0.013291000000
H	3.314235000000	-2.335350000000	0.000060000000
H	2.797747000000	1.982860000000	-0.029447000000
H	4.366443000000	-0.013117000000	-0.030912000000
N	1.092654000000	0.798271000000	-0.000142000000
H	-3.869116000000	0.906386000000	-0.103241000000
H	-4.006222000000	-1.829368000000	0.037920000000
O	-0.478232000000	2.992753000000	-0.035585000000

H	-0.673063000000	3.310407000000	0.858050000000
H	0.512335000000	1.683837000000	0.012757000000

Va →Vb TS 1^1A -532.12197a.u.
RC mode i1140

C	-3.112402000000	-1.169141000000	0.012384000000
C	-3.053435000000	0.242313000000	-0.059593000000
C	-1.781356000000	-1.621251000000	0.052807000000
C	-0.964714000000	-0.453979000000	0.005579000000
N	-1.763654000000	0.673603000000	-0.064405000000
H	-1.444278000000	-2.657943000000	0.111988000000
H	-1.206403000000	1.922893000000	-0.080265000000
C	0.474246000000	-0.381332000000	0.004602000000
C	1.299624000000	-1.541572000000	0.014758000000
C	2.686173000000	-1.429069000000	0.005234000000
C	2.445771000000	0.958426000000	-0.027518000000
C	3.285737000000	-0.149680000000	-0.019333000000
H	0.823381000000	-2.524772000000	0.025369000000
H	3.306422000000	-2.331383000000	0.011595000000
H	2.824737000000	1.985327000000	-0.048467000000
H	4.370359000000	-0.019832000000	-0.032899000000
N	1.098246000000	0.836472000000	-0.012208000000
H	-3.877898000000	0.957325000000	-0.111043000000
H	-4.016086000000	-1.780799000000	0.031375000000
O	-0.458637000000	2.777850000000	-0.023745000000
H	-0.558555000000	3.089278000000	0.888760000000
H	0.427405000000	1.838278000000	-0.003676000000

(VIa) Quinoline -Water(M^0•H_2O) 1^1A -608.16486a.u.

C	-2.994395000000	-0.915579000000	-0.009338000000
C	-3.074738000000	0.474744000000	-0.041219000000
C	-1.601612000000	-1.243775000000	0.006860000000
C	-0.889519000000	-0.006265000000	-0.014480000000
N	-1.805910000000	1.010977000000	-0.044906000000
H	-1.555501000000	2.013467000000	-0.053499000000
C	0.538108000000	0.053515000000	-0.014977000000
C	1.236349000000	-1.207904000000	0.014666000000
C	2.653561000000	-1.159011000000	0.013324000000
C	2.523100000000	1.252009000000	-0.045622000000
C	3.302056000000	0.072448000000	-0.017325000000
H	3.224427000000	-2.095086000000	0.035092000000
H	3.009415000000	2.235043000000	-0.072541000000
H	4.394181000000	0.139659000000	-0.020827000000
N	1.183675000000	1.260213000000	-0.043508000000
H	-3.948346000000	1.126687000000	-0.063293000000
H	-3.837178000000	-1.606938000000	-0.001476000000
C	0.510012000000	-2.449026000000	0.040820000000

H	1.081597000000	-3.383763000000	0.062714000000
C	-0.874226000000	-2.472028000000	0.036660000000
H	-1.410141000000	-3.427922000000	0.054535000000
O	-0.539415000000	3.508507000000	0.002372000000
H	-0.457287000000	3.779196000000	0.927523000000
H	0.197620000000	2.858503000000	-0.084516000000

(VIb) Quinoline -Water(M^1•H_2O) 1^1A --608.14272a.u.

C	-3.049628000000	-0.768652000000	-0.007397000000
C	-3.030623000000	0.639242000000	-0.040735000000
C	-1.688783000000	-1.166970000000	0.011163000000
C	-0.940320000000	0.074205000000	-0.010980000000
N	-1.761379000000	1.164557000000	-0.042968000000
H	-1.013320000000	2.691433000000	-0.098311000000
C	0.476429000000	0.028665000000	-0.005827000000
C	1.154235000000	-1.255015000000	0.010032000000
C	2.566600000000	-1.249596000000	0.002556000000
C	2.587181000000	1.161619000000	-0.030527000000
C	3.288213000000	-0.049871000000	-0.021124000000
H	3.097433000000	-2.209009000000	0.013319000000
H	3.071271000000	2.141458000000	-0.046492000000
H	4.380730000000	-0.040847000000	-0.030401000000
N	1.241302000000	1.165774000000	-0.021097000000
H	-3.894251000000	1.310187000000	-0.066353000000
H	-3.930980000000	-1.412643000000	-0.000834000000
C	0.381714000000	-2.461878000000	0.032985000000
H	0.912637000000	-3.419586000000	0.046116000000
C	-1.007606000000	-2.415468000000	0.033626000000
H	-1.578322000000	-3.352346000000	0.049522000000
O	-0.268258000000	3.368322000000	-0.015914000000
H	-0.412488000000	3.712968000000	0.877400000000
H	0.729419000000	2.101794000000	-0.010837000000

VIa →VIb TS 1^1A -608.13842a.u.
RC mode i1153

C	-3.045306000000	-0.745198000000	-0.011933000000
C	-3.035495000000	0.658025000000	-0.045401000000
C	-1.679863000000	-1.144467000000	0.009637000000
C	-0.925845000000	0.083349000000	-0.009804000000
N	-1.757973000000	1.167005000000	-0.045100000000
H	-1.121301000000	2.389879000000	-0.053600000000
C	0.497673000000	0.053803000000	-0.007839000000
C	1.164700000000	-1.230050000000	0.012410000000
C	2.579567000000	-1.224691000000	0.005284000000
C	2.574281000000	1.188937000000	-0.039364000000
C	3.288869000000	-0.021419000000	-0.023273000000
H	3.114982000000	-2.181611000000	0.019930000000
H	3.071970000000	2.163839000000	-0.061423000000
H	4.381985000000	-0.005565000000	-0.032357000000
N	1.232587000000	1.209490000000	-0.030331000000
H	-3.892746000000	1.335365000000	-0.072399000000
H	-3.925757000000	-1.389801000000	-0.007387000000
C	0.389720000000	-2.437729000000	0.036959000000

H	0.920275000000	-3.395939000000	0.053200000000
C	-0.998328000000	-2.395254000000	0.035367000000
H	-1.568942000000	-3.331885000000	0.051065000000
O	-0.298753000000	3.166049000000	-0.004298000000
H	-0.351078000000	3.483332000000	0.910380000000
H	0.578495000000	2.256687000000	-0.01726100000

(VIIa) Formamide (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -245.68054

C	-1.198876000000	-0.166730000000	0.009008000000
N	-0.689448000000	1.088301000000	0.021856000000
H	0.327742000000	1.184704000000	-0.042404000000
H	-2.312390000000	-0.189804000000	0.023205000000
H	-1.300868000000	1.889534000000	-0.055058000000
O	-0.529179000000	-1.200592000000	-0.002232000000
O	1.985159000000	0.093946000000	-0.095381000000
H	2.352910000000	-0.042344000000	0.787883000000
H	1.304164000000	-0.606648000000	-0.139772000000

(VIIb) Formamide (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -245.66671

C	1.186330000000	-0.064887000000	0.017334000000
N	0.653557000000	1.109535000000	-0.005613000000
H	-0.481057000000	-0.918443000000	-0.045383000000
H	2.268350000000	-0.271584000000	0.055413000000
H	1.394168000000	1.816113000000	0.010426000000
O	0.476348000000	-1.191272000000	-0.002388000000
O	-1.899382000000	0.070762000000	-0.091994000000
H	-2.260924000000	0.170850000000	0.799723000000
H	-1.229146000000	0.789721000000	-0.129835000000

(VIIa)-(VIIb) TS 1^1A -245.64926a.u.
RC mode i1575

C	1.084173000000	-0.118144000000	0.016494000000
N	0.547578000000	1.085138000000	0.000241000000
H	-0.753455000000	0.862382000000	-0.062542000000
H	2.182131000000	-0.245840000000	0.046810000000
H	1.215203000000	1.852242000000	0.000027000000
O	0.374030000000	-1.187830000000	-0.002931000000
O	-1.646755000000	0.095775000000	-0.099391000000
H	-2.019389000000	0.099402000000	0.795507000000
H	-0.780779000000	-0.718849000000	-0.061874000000

(VIIIa) 2-hydroxyl-pyridine (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -398.83623

H	2.697963000000	0.250034000000	-0.133628000000
O	1.274368000000	1.434100000000	-0.026859000000
N	0.277329000000	-0.640520000000	-0.022971000000
C	-2.229420000000	0.466247000000	0.025545000000
C	-1.122774000000	1.291094000000	0.016857000000
C	0.227558000000	0.758786000000	-0.010765000000

C	-0.806307000000	-1.469027000000	-0.016387000000
C	-2.083834000000	-0.953623000000	0.007770000000
H	-3.231594000000	0.908641000000	0.044670000000
H	-0.589640000000	-2.540709000000	-0.032409000000
H	-2.946048000000	-1.622558000000	0.012075000000
H	-1.216324000000	2.380270000000	0.028199000000
O	3.068398000000	-0.657628000000	-0.059186000000
H	1.238911000000	-1.020870000000	-0.036306000000
H	3.451962000000	-0.643807000000	0.828436000000

(VIIIb) 2-hydroxyl-pyridine (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -398.83932

H	2.052474000000	0.802530000000	-0.064304000000
O	1.267213000000	1.407986000000	-0.032918000000
N	0.304621000000	-0.702922000000	-0.037340000000
C	-2.242420000000	0.487191000000	0.034470000000
C	-1.093080000000	1.275498000000	0.019706000000
C	0.168206000000	0.636844000000	-0.016550000000
C	-0.823071000000	-1.452847000000	-0.024242000000
C	-2.111106000000	-0.915473000000	0.011595000000
H	-3.231083000000	0.957065000000	0.061866000000
H	-0.669042000000	-2.537961000000	-0.044293000000
H	-2.984309000000	-1.573070000000	0.020364000000
H	-1.133026000000	2.367737000000	0.034209000000
O	3.091833000000	-0.593161000000	-0.049285000000
H	2.218462000000	-1.038543000000	-0.106174000000
H	3.350648000000	-0.763169000000	0.867470000000

(VIIIa)-(VIIIb) TS 1^1A -398.81696a.u.
RC mode i1528

H	2.277777000000	0.408213000000	-0.064165000000
O	1.402713000000	1.325640000000	-0.023935000000
N	0.319057000000	-0.697150000000	-0.022845000000
C	-2.152170000000	0.555337000000	0.023248000000
C	-0.992190000000	1.317684000000	0.014223000000
C	0.285816000000	0.676611000000	-0.009043000000
C	-0.813650000000	-1.440609000000	-0.016476000000
C	-2.074166000000	-0.858981000000	0.006978000000
H	-3.128427000000	1.051999000000	0.040478000000
H	-0.673696000000	-2.526609000000	-0.032372000000
H	-2.969973000000	-1.484004000000	0.011199000000
H	-1.014705000000	2.410493000000	0.023662000000
O	2.737407000000	-0.663945000000	-0.067018000000
H	1.564793000000	-0.993211000000	-0.041718000000
H	3.068037000000	-0.780646000000	0.836877000000

(IXa) piperidine-2-one (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -402.40735

C	-2.172019000000	0.489430000000	0.372993000000
C	-1.014123000000	1.388210000000	-0.073620000000

C	0.351494000000	0.714349000000	-0.054614000000
N	0.389507000000	-0.642085000000	-0.051567000000
C	-0.744937000000	-1.549273000000	0.089549000000
C	-2.057706000000	-0.876987000000	-0.306703000000
H	-3.136673000000	0.967573000000	0.139066000000
H	-2.144230000000	0.356291000000	1.469987000000
H	-0.929303000000	2.301841000000	0.533137000000
H	-1.171903000000	1.726586000000	-1.113891000000
H	1.343549000000	-1.025014000000	-0.022466000000
H	-0.559607000000	-2.437716000000	-0.536064000000
H	-0.814468000000	-1.906853000000	1.136209000000
H	-2.897431000000	-1.534541000000	-0.030518000000
H	-2.091481000000	-0.747621000000	-1.403339000000
O	1.386192000000	1.395811000000	-0.085842000000
O	3.253083000000	-0.628491000000	-0.009115000000
H	2.822700000000	0.252839000000	-0.126414000000
H	3.561844000000	-0.591727000000	0.909282000000

(IXb) piperidine-2-ol (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -402.39231

C	0.741422000000	-1.534323000000	0.095631000000
C	0.983863000000	1.375289000000	-0.047879000000
C	-0.312440000000	0.598130000000	-0.028546000000
N	-0.444725000000	-0.678932000000	0.034118000000
C	2.183227000000	0.502721000000	0.334510000000
C	2.048714000000	-0.864560000000	-0.338921000000
H	0.543874000000	-2.424685000000	-0.524920000000
H	0.840668000000	-1.909627000000	1.133159000000
H	0.868860000000	2.246490000000	0.616246000000
H	1.101569000000	1.786513000000	-1.066939000000
H	3.124046000000	1.000829000000	0.051822000000
H	2.211596000000	0.369179000000	1.431128000000
H	2.901218000000	-1.518342000000	-0.091374000000
H	2.049957000000	-0.734673000000	-1.436672000000
O	-1.384940000000	1.397856000000	-0.100820000000
H	-2.199509000000	0.818083000000	-0.115690000000
O	-3.174494000000	-0.603163000000	-0.044132000000
H	-2.258865000000	-0.994569000000	-0.040779000000
H	-3.463586000000	-0.707762000000	0.876037000000

(IXa)-(IXb) TS 1^1A -402.37935a.u.
RC mode i1502

C	0.739238000000	-1.527677000000	0.104195000000
C	0.896428000000	1.406465000000	-0.053847000000
C	-0.397761000000	0.625591000000	-0.025266000000
N	-0.450703000000	-0.685070000000	0.039140000000
C	2.113593000000	0.557915000000	0.329378000000
C	2.016035000000	-0.813269000000	-0.344565000000
H	0.559071000000	-2.421126000000	-0.516653000000
H	0.863724000000	-1.894979000000	1.141856000000

H	0.770537000000	2.284851000000	0.597912000000
H	1.000743000000	1.804669000000	-1.079305000000
H	3.043447000000	1.076458000000	0.047041000000
H	2.146028000000	0.424856000000	1.425992000000
H	2.891128000000	-1.439215000000	-0.105492000000
H	2.000735000000	-0.683549000000	-1.441972000000
O	-1.493323000000	1.316425000000	-0.092906000000
H	-2.351665000000	0.503251000000	-0.093341000000
O	-2.883504000000	-0.645950000000	-0.052929000000
H	-1.710868000000	-0.976155000000	0.016058000000
H	-3.248540000000	-0.741519000000	0.841227000000

(Xa) Isoxazoline (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -396.65157

C	1.470829000000	0.968084000000	0.024949000000
C	2.128973000000	-0.233801000000	0.020269000000
O	1.252206000000	-1.261306000000	-0.010698000000
N	-0.034384000000	-0.748082000000	-0.026175000000
H	-1.761151000000	0.841694000000	-0.052934000000
H	1.884814000000	1.972853000000	0.045228000000
H	3.180858000000	-0.515081000000	0.035478000000
C	0.095557000000	0.580710000000	-0.006354000000
O	-0.950757000000	1.414395000000	-0.018495000000
O	-2.815182000000	-0.540591000000	-0.064507000000
H	-2.029656000000	-1.112009000000	-0.167750000000
H	-3.096471000000	-0.740814000000	0.839614000000

(Xb) Isoxazoline (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -396.63754

C	-1.495715000000	0.934910000000	-0.106665000000
C	-2.049202000000	-0.307371000000	-0.150416000000
O	-1.151627000000	-1.303634000000	0.039388000000
N	0.048909000000	-0.647589000000	0.321793000000
H	0.891276000000	-1.147464000000	-0.000083000000
H	-1.994561000000	1.889640000000	-0.252935000000
H	-3.073015000000	-0.652806000000	-0.293484000000
C	-0.059681000000	0.727623000000	0.093496000000
O	0.899501000000	1.507251000000	0.098001000000
O	2.731866000000	-0.614991000000	-0.270560000000
H	3.237485000000	-0.695034000000	0.549524000000
H	2.386111000000	0.298811000000	-0.208688000000

(Xa)-(Xb) TS 1^1A -396.61971a.u.
RC mode i1325

C	1.392225000000	1.003036000000	0.006038000000
C	2.040249000000	-0.200043000000	-0.005296000000
O	1.178415000000	-1.246310000000	-0.002889000000
N	-0.084194000000	-0.695120000000	0.021943000000
H	-2.033962000000	0.382966000000	-0.083344000000
H	1.829145000000	1.998450000000	0.002312000000

H	3.092599000000	-0.481058000000	-0.014719000000
C	-0.016735000000	0.660242000000	0.012714000000
O	-1.072192000000	1.384355000000	0.000012000000
O	-2.442947000000	-0.638240000000	-0.105304000000
H	-1.290928000000	-1.055364000000	-0.058788000000
H	-2.808134000000	-0.757002000000	0.785642000000

(XIa) Cytosine (M^0) – H2O ($M^0 \bullet H_2O$) 1^1A -470.08000

H	3.028570000000	-0.556037000000	-0.136866000000
O	1.436314000000	-1.500493000000	-0.031168000000
N	0.784223000000	0.688206000000	-0.018679000000
C	-1.764130000000	-0.132686000000	0.012040000000
C	0.499528000000	-0.693321000000	-0.013606000000
C	-0.178478000000	1.643233000000	-0.017661000000
C	-1.500769000000	1.282838000000	-0.000059000000
H	0.161224000000	2.683005000000	-0.028135000000
H	-2.296487000000	2.028888000000	0.016547000000
N	-0.827440000000	-1.068845000000	-0.000197000000
N	-3.068385000000	-0.562810000000	0.098951000000
H	-3.181805000000	-1.548326000000	-0.125612000000
H	-3.776909000000	0.047796000000	-0.294339000000
O	3.539490000000	0.279786000000	-0.054194000000
H	1.790534000000	0.917828000000	-0.027475000000
H	3.912744000000	0.196266000000	0.833965000000

(XIb) Cytosine (M^1) – H2O ($M^1 \bullet H_2O$) 1^1A -470.08269

H	2.282577000000	-1.005055000000	-0.068260000000
O	1.412301000000	-1.479235000000	-0.040708000000
N	0.829991000000	0.750281000000	-0.035999000000
C	-1.783107000000	-0.121326000000	0.017440000000
C	0.456660000000	-0.548884000000	-0.022248000000
C	-0.186407000000	1.640927000000	-0.026612000000
C	-1.523781000000	1.271151000000	0.003240000000
H	0.101699000000	2.698745000000	-0.041934000000
H	-2.324962000000	2.013686000000	0.021120000000
N	-0.797428000000	-1.030232000000	0.000495000000
N	-3.067266000000	-0.615653000000	0.112795000000
H	-3.132993000000	-1.596573000000	-0.148525000000
H	-3.797463000000	-0.032749000000	-0.284253000000
O	3.554973000000	0.188040000000	-0.039076000000
H	2.768733000000	0.773346000000	-0.095007000000
H	3.826931000000	0.296176000000	0.883178000000

(XIa)-(XIb) TS 1^1A -470.06035a.u.
RC mode i1526

H	2.539921000000	-0.723337000000	-0.065055000000
O	1.507202000000	-1.450038000000	-0.030084000000
N	0.852457000000	0.731435000000	-0.018711000000
C	-1.716584000000	-0.140261000000	0.012102000000

C	0.535165000000	-0.614121000000	-0.011943000000
C	-0.141632000000	1.643870000000	-0.018117000000
C	-1.469108000000	1.264699000000	-0.000069000000
H	0.161366000000	2.696583000000	-0.030257000000
H	-2.275763000000	2.000234000000	0.013313000000
N	-0.748243000000	-1.058524000000	0.001275000000
N	-3.005843000000	-0.615175000000	0.096924000000
H	-3.086092000000	-1.599797000000	-0.144915000000
H	-3.732623000000	-0.023651000000	-0.292462000000
O	3.214356000000	0.232951000000	-0.062146000000
H	2.128176000000	0.783333000000	-0.034749000000
H	3.556912000000	0.274066000000	0.843707000000

(4) Calculations for figure 3

A) Energies for the geometry optimized structures (B3LYP/aug-cc-pVDZ)

Absolute energies (in Hartree) of the tautomers and water complexes of 2-Hydroxypyridine and 2-piperidone. ΔE is the energy (in kcal/mol) relative to the keto-form, including BSSE correction for the water complexes. The BSSE correction (in kcal/mol) is also shown.

Calculation HB energies and the BSSE corrections:

	pyridine-enol	pyridine-keto	piperidine-enol	piperidine-keto
AB(opt)	-400.0316409372	-400.0341678011	-402.440645713	-402.4573126715
A(opt)	-323.5703581245	-323.5709113040	-325.978191991	-325.9962228448
B(opt)	-76.4461832713	-76.4461832713	-76.4461832713	-76.4461832713
ΔE(HB)-uncorr	-9.47	-10.71	-10.21	-9.35
BSSE-correction: calculated geometries of the complexes fixed				
A	-323.5695471391	-323.5703581932	-325.9773443664	-325.9957731730
A + Bghost	-323.5699651536	-323.5707150842	-325.9777807664	-325.9961002787
B	-76.4457304604	-76.4456899279	-76.4454611065	-76.4457828732
B + Aghost	-76.4461891294	-76.4460449703	-76.4459338584	-76.4461167363
BSSE	0.0008766835	0.0007119334	0.0009091519	0.0006609688
corrected HB energies (kcal/mole)				
BSSE	0.55	0.45	0.57	0.41
ΔE(HB)	-8.92	-10.27	-9.64	-8.94
ΔΔE(HB)		-1.34		0.70

Calculation of the BSSE correction for the four complexes. AB(opt), A(opt), and B(opt) refer to the optimized structures of the complex AB and the two fragments A and B. The differences of these energies gives the uncorrected HB energies. For the BSSE correction, the separated fragments were calculated with their own basis functions, and with the ghost-orbitals of the other fragment present – all in the fixed geometry of the complex.

(5) Table T1. Dipole moments μ^0 (in D) and μ^1 (in D) of M^0 and M^1 tautomers and H-bonding energy ΔE_{HB} of the cyclic monohydrates $M^0 \bullet H_2O$ and $M^1 \bullet H_2O$ (in kcal/mol), correspondingly, for compounds I-XI.

	I	II	III	IV	V	VI	VII	VIII	IX	X	XI
μ^0 (D)	1.6	1.9	2.1	3.7	1.0	0.4	3.8	4.0	3.8	2.4	6.0
μ^1 (D)	3.6	2.4	2.2	5.1	4.9	5.1	0.9	1.0	1.2	1.6	3.0
$\Delta E_{HB}(M^0)$	16.5	14.0	13.5	12.8	14.5	17.0	14.2	16.5	14.7	14.7	17.0
$\Delta E_{HB}(M^1)$	19.0	18.2	17.8	17.7	19.8	23.4	17.5	16.1	16.9	16.9	16.3

(6) Table T2. Calculated NICS(1)zz indexes (B3LYP/cc-pVDZ level of theory at points 1 Å above the centers of the aromatic rings) for compounds II,III,VIII,X and XI and their water complexes in both tautomeric forms M^0 and M^1.

	NICS(1)zz			NICS(1)zz	
	M^0	M^1		M^0	M^1
II	-22.7	-2.8	**VIII**	-10.6	-24.5
II-H_2O	-20.8	-6.9	VIII-H_2O	-13.2	-23.0
ΔNICS(1)zz	+1.9	-4.1	ΔNICS(1)zz	-2.6	+1.5
III	-22.3	-2.5	**X**	-22.4	-12.2
III-H_2O	-20.6	-6.2	X-H_2O	-22.1	-14.8
ΔNICS(1)zz	+1.7	-3.7	ΔNICS(1)zz	+0.3	-2.6
			XI	-5.5	-17.1
			XI-H_2O	-6.9	-15.2
			ΔNICS(1)zz	-1.4	+1.9

7)

Table T3. The relative energy of monomers in ground state S0 Erel(M)(in kcal/mol) and in excited state S_1 E_{rel}(M*)(in kcal/mol); the relative energy of water complexes M•H2O in ground state S0 Erel(M•H2O) (in kcal/mol) and in excited state S1 Erel(M•H2O)* (in kcal/mol); HB stabilization energy of water complexes M•H2O in ground state S0 EHB(M•H2O) (in kcal/mol) and in excited state S1 EHB(M•H2O)* (in kcal/mol).

Relative energy	I		II		III		V		VI	
	M^0	M^1	M^0	M^1	M^0	M^1	M^0	M^1	M^0	M^1

(kcal/mol)										
E_{rel}(M)	0.0	12.6	0.0	14.0	0.0	14.9	0.0	17.5	0.0	18.8
E_{rel}(M*)	23.8	0.0	15.9	0.0	4.7	0.0	23.8	0.0	17.5	0.0
E_{rel}(M•H_2O)	0.0	8.5	0.0	9.8	0.0	10.6	0.0	12.2	0.0	12.4
E_{rel}(M•H_2O)*	17.8	0.0	11.9	0.0	6.3	0.0	24.5	0.0	12.3	0.0
E_{HB}(M•H_2O)	16.5	19.0	14.0	18.2	13.5	17.8	17.5	19.8	18.8	23.4
E_{HB}(M•H_2O)*	20.6	14.7	18.9	14.9	14.0	14.9	21.4	29.3	22.8	17.7

[i] Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.