Supplementary Material for:

The importance of Specific Solvent-Solute Interactions for Studying UV-Vis Spectra of Light-Responsive Molecular Switches

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**Table S1**. Difference in electronic energy, enthalpy, Gibbs free energy between deZ and deE-isomer structure for different functionals.

|  |  |  |
| --- | --- | --- |
| Functional | Enthalpy  [kcal/mol] | Gibbs free energy  [kcal/mol] |
| cam-B3LYP | 5.8 | 3.8 |
| B3LYP | 7.8 | 5.6 |
| M062X | 21.1 | 16.7 |
| PB1PBE | 10.2 | 8.0 |

**Table S2.** Wavelength and orbitals involved in electronic transitions for two basis sets and wavelength for experimental (Only transitions with the oscillatory strength higher than 0.05 and contribution percentage higher than 41% are included.)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | basis set/experimental | wavelenght [nm] | transitions | Oscillatory strength |
| deE-isomer | cc-pVDZ | 461 | HOMO→LUMO (90%) | 0.3382 |
| 343 | HOMO→LUMO+1 (41%) | 0.1023 |
| HOMO→LUMO+2 (50%) |
| 296 | HOMO-2→LUMO (85%) | 0.1414 |
| cc-pVTZ | 452 | HOMO→LUMO (88%) | 0.3194 |
| 340 | HOMO→LUMO+2 (66%) | 0.0985 |
| 292 | HOMO-2→LUMO (82%) | 0.01634 |
| experimental | 400 | | |
| 325 | | |
| 288 | | |
| deZ-isomer | cc-pVDZ | 325 | HOMO→LUMO+2 (76%) | 0.1144 |
| 276 | HOMO-2→LUMO (47%) | 0.0518 |
| cc-pVTZ | 323 | HOMO→LUMO+1 (83%) | 0.1122 |
| 272 | HOMO-2→LUMO (60%) | 0.0866 |
| experimental | 300 | | |
| 275 | | |

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**Figure S3.** Selected orbitals included in the electronic transition of deZ-isomer a) HOMO and b) LUMO.

**Table S4.** Calculated electronic transitions of deE-isomer with 5 solvent molecules.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Experimental [nm] | wavelength [nm] | Transitions | Oscillatory strength |
| E-isomer | 330 | 292 | HOMO→LUMO (78%) | 0.3598 |
| 250 | 253 | HOMO-1→LUMO (61%) | 0.3834 |
| 240 | 238 | Multiple transitions | 0.0506 |
| Z-isomer | 265 | 261 | Multiple transitions | 0.0719 |
| 254 | Multiple transitions | 0.1415 |
| deE-isomer | 400 | 402 | HOMO→LUMO (72%) | 0.3726 |
| 325 | 323 | HOMO→LUMO+2 (69%) | 0.0307 |
| 283 | 273 | HOMO-2→LUMO (68%) | 0.2064 |
| deZ-isomer | 285 | 304 | HOMO→LUMO (52%) | 0.0894 |
| 262 | Multiple transitions | 0.0639 |
| 250 | HOMO-1→LUMO (56%) | 0.2093 |

**Table S5.** Change in electronic enthalpy and Gibbs free energy of structures 1-4.

|  |  |  |
| --- | --- | --- |
| deE+1H2O | Enthalpy  [kJ/mol] | Gibbs free energy  [kJ/mol] |
| 1 | -61 | -25 |
| 2 | -46 | -9.6 |
| 3 | -46 | -9.6 |
| 4 | -33 | 0 |

**Table S6.** Charges on specific atoms due to the presence of water molecule.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | 1 | 2 | 3 | 4 |
| Ophen | -0.804 | -0.762 | -0.763 | -0.765 |
| N1 | -0.311 | -0.353 | -0.350 | -0.331 |
| N2 | -0.428 | -0.415 | -0.415 | -0.420 |
| Ocarb | -0.612 | -0.651 | -0.652 | -0.619 |
| Npyr | -0.437 | -0.436 | -0.436 | -0.487 |
| Owater | -0.985 | -0.967 | -0.967 | -0.958 |

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**Figure S7.** Electronic spectra of structures 1-4 and deE+5H2O.

**Table S8.** Electron density (in units a.u.) and Laplacian (in units a.u.) at BCP and bond lengths (in Å) of selected bonds influenced by the explicit solvent effect.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | deE-isomer | Structure 1 | Structure 2 | Structure 3 | Structure 4 | E-isomer | Z-isomer | deE-isomer | deZ-isomer |
| O-C | 0.3827 | 0.3685 | 0.3841 | 0.3839 | 0.3831 | 0.3088 | 0.2992 | 0.3734 | 0.3499 |
| -0.6748 | -0.7023 | -0.6680 | -0.6689 | -0.6718 | -0.5880 | -0.5568 | -0.6850 | -0.5606 |
| 1.2587 | 1.2748 | 1.2570 | 1.2572 | 1.2580 | 1.3438 | 1.3548 | 1.2687 | 1.2974 |
| O—H (methyl group) | 0.0282 | / | 0.0270 | 0.0268 | 0.0287 | / | / | 0.0233 | / |
| 0.1050 | 0.1024 | 0.1017 | 0.1064 | 0.0931 |
| 1.9951 | 2.0182 | 2.0207 | 1.9845 | 2.100 |
| O—H | / | 0.0508 | / | / | / | 0.0279 | 0.0205 | 0.0476 | 0.0398 |
| 0.0983 | 0.0882 | 0.0716 | 0.0978 | 0.0943 |
| 1.6754 | 1.8800 | 2.0507 | 1.7012 | 1.7741 |
| H—N (immino group) | / | / | 0.0079 | 0.0078 | / | / | / | 0.0228 | / |
| 0.0271 | 0.0256 | 0.0614 |
| 2.6891 | 2.6986 | 2.0700 |
| H—O | / | / | 0.0264 | 0.0262 | / | 0.0235 | 0.0407 | 0.0160 | / |
| 0.0832 | 0.0829 | 0.0877 | 0.0996 | 0.0620 |
| 1.9141 | 1.9166 | 1.9172 | 1.7517 | 1.9130 |
| C=O | 0.4216 | 0.4231 | 0.4157 | 0.4156 | 0.4215 | 0.4238 | 0.4120 | 0.4137 | 0.4204 |
| -0.5042 | -0.4937 | -0.5326 | -0.5333 | -0.5066 | -0.4400 | -0.5334 | -0.5369 | -0.4787 |
| 1.2152 | 1.2135 | 1.2211 | 1.2211 | 1.2154 | 1.2105 | 1.2252 | 1.2228 | 1.2153 |
| H—N | / | / | / | / | 0.0352 | 0.0297 | 0.0302 | 0.0337 | 0.0360 |
| 0.0725 | 0.0736 | 0.0732 | 0.0730 | 0.0720 |
| 1.8920 | 1.9566 | 1.9500 | 1.9087 | 1.8852 |
| N-C | 0.3533 | 0.3534 | 0.3535 | 0.3535 | 0.3513 | 0.3523 | 0.3520 | 0.3513 | 0.3515 |
| -1.0475 | -1.0475 | -1.0473 | -1.0476 | -1.0246 | -1.1016 | -1.0244 | -1.0212 | -1.0182 |
| 1.3269 | 1.3267 | 1.3268 | 1.3269 | 1.3280 | 1.3286 | 1.3300 | 1.3274 | 1.3300 |
| N-C | 0.3557 | 0.3559 | 0.3558 | 0.3558 | 0.3536 | 0.3535 | 0.3549 | 0.3541 | 0.3529 |
| -1.0542 | -1.0541 | -1.0553 | -1.0550 | -1.0312 | -1.0385 | -1.0268 | -1.0318 | -1.1021 |
| 1.3300 | 1.3230 | 1.3230 | 1.3230 | 1.3305 | 1.3289 | 1.3258 | 1.3304 | 1.3282 |

The Cartesian coordinates for the optimized deE and deZ isomers with different functionals

**deE optimized at CAM-B3LYP/cc-pVDZ**

Symbol X Y Z

C 3.8961800 0.9983820 0.0819990

C 2.8017480 0.0332960 0.0100410

C 3.0966770 -1.3459200 -0.0846370

C 4.3804450 -1.8469210 -0.1141490

C 5.4559940 -0.9336870 -0.0464610

C 5.2236060 0.4130520 0.0464420

C 1.3883550 0.4213710 0.0293360

C 1.0002900 1.8773170 0.1576950

O 3.7818670 2.2528930 0.1681790

N 0.4888080 -0.5150260 -0.0655040

N -0.8151310 -0.0922720 -0.0404070

C -1.8509200 -0.9648180 -0.0713680

O -1.7631410 -2.1816830 -0.1138060

C -3.2131530 -0.3061710 -0.0382650

C -3.4811670 1.0215880 -0.3754820

C -4.7939680 1.4807260 -0.3159670

N -5.8350630 0.7286870 0.0441820

C -5.5699340 -0.5453150 0.3499310

C -4.2993200 -1.1046810 0.3170850

H 6.4869810 -1.3046160 -0.0677590

H 4.5592170 -2.9217110 -0.1869450

H 2.2447580 -2.0258560 -0.1346400

H 6.0441170 1.1333380 0.0998330

H 1.9201390 2.4782370 0.1940180

H 0.3792250 2.1924910 -0.7001990

H 0.4128780 2.0458800 1.0788990

H -1.0136170 0.8869080 0.1382760

H -4.1187190 -2.1530810 0.5528540

H -6.4314410 -1.1573420 0.6366900

H -5.0193780 2.5188750 -0.5811780

H -2.6932630 1.6981550 -0.7099400

**deE optimized at B3LYP/cc-pVDZ**

Symbol X Y Z

C 3.9198600 0.9998380 0.0791610

C 2.8065670 0.0365390 0.0083760

C 3.0983230 -1.3512140 -0.0885040

C 4.3852340 -1.8569810 -0.1203070

C 5.4733650 -0.9502420 -0.0535240

C 5.2485730 0.4033920 0.0413010

C 1.3980830 0.4344670 0.0315530

C 1.0113730 1.8960450 0.1600660

O 3.8151160 2.2588040 0.1658900

N 0.4869270 -0.5093550 -0.0617020

N -0.8148820 -0.0917090 -0.0378260

C -1.8611290 -0.9687160 -0.0571760

O -1.7648210 -2.1934850 -0.0804100

C -3.2208690 -0.3071100 -0.0336630

C -3.4944960 1.0326280 -0.3557230

C -4.8131600 1.4902330 -0.3056450

N -5.8663830 0.7304860 0.0304180

C -5.5969820 -0.5534510 0.3212790

C -4.3208780 -1.1128830 0.2970810

H 6.5018340 -1.3310800 -0.0770330

H 4.5580160 -2.9339740 -0.1943350

H 2.2450970 -2.0305160 -0.1377840

H 6.0753130 1.1182430 0.0938690

H 1.9291760 2.4999440 0.2021740

H 0.3951630 2.2176380 -0.7016490

H 0.4154250 2.0674300 1.0774380

H -1.0174630 0.8941020 0.1128140

H -4.1444880 -2.1652140 0.5224210

H -6.4611930 -1.1729930 0.5880450

H -5.0355720 2.5332550 -0.5591660

H -2.7064800 1.7193760 -0.6725210

**deE optimized at M062X/cc-pVDZ**

Symbol X Y Z

C 3.8915960 1.0073110 0.0317020

C 2.7987740 0.0346700 0.0264350

C 3.0927290 -1.3489640 0.0005120

C 4.3781660 -1.8509800 -0.0148960

C 5.4543390 -0.9331030 -0.0062580

C 5.2213730 0.4180830 0.0172840

C 1.3843140 0.4217130 0.0375260

C 0.9829160 1.8690550 0.2285390

O 3.7757060 2.2614500 0.0407420

N 0.4873580 -0.5134540 -0.1022290

N -0.8153830 -0.0949960 -0.0543150

C -1.8477670 -0.9719130 -0.1282760

O -1.7590430 -2.1821290 -0.2378370

C -3.2085720 -0.3105720 -0.0552170

C -3.4704670 1.0305040 -0.3463650

C -4.7823240 1.4940580 -0.2547670

N -5.8249120 0.7356080 0.0939520

C -5.5626930 -0.5507900 0.3532940

C -4.2940570 -1.1179190 0.2858440

H 6.4848430 -1.3033670 -0.0161410

H 4.5567130 -2.9269940 -0.0285390

H 2.2419450 -2.0322870 -0.0030330

H 6.0418850 1.1394370 0.0232510

H 1.8857950 2.4886570 0.2628820

H 0.3392120 2.2017710 -0.6046350

H 0.4101890 1.9852570 1.1662430

H -1.0236730 0.8649090 0.2036550

H -4.1168430 -2.1745590 0.4843630

H -6.4243740 -1.1656080 0.6294140

H -5.0064290 2.5401140 -0.4832270

H -2.6819590 1.7110830 -0.6714660

**deE optimized at PBE1PBE/cc-pVDZ**

Symbol X Y Z

C 3.8888610 1.0044320 0.0781800

C 2.7913570 0.0346990 0.0082660

C 3.0894430 -1.3461560 0.0848000

C 4.3759640 -1.8434450 -0.1139260

C 5.4519160 -0.9293990 -0.0477880

C 5.2164980 0.4195990 0.0435290

C 1.3847620 0.4191220 0.0286860

C 0.9928740 1.8702850 0.1511410

O 3.7732900 2.2579270 0.1616570

N 0.4830260 -0.5265760 -0.0615250

N -0.8069040 -0.1101420 -0.0389620

C -1.8510180 -0.9771320 -0.0594540

O -1.7660700 -2.1978630 -0.0841250

C -3.1995260 -0.3067820 -0.0348360

C -3.4616450 1.0322230 -0.3476550

C -4.7742950 1.4949740 -0.2947640

N -5.8278470 0.7427700 0.0350360

C -5.5681970 -0.5393280 0.3164230

C -4.2994890 -1.1060800 0.2892420

H 6.4835320 -1.2997980 -0.0689070

H 4.5563050 -2.9185810 -0.1853700

H 2.2372360 -2.0276600 -0.1334540

H 6.0375650 1.1402450 0.0955860

H 1.9139370 2.4731580 0.1936890

H 0.3812780 2.1869380 -0.7142010

H 0.3962260 2.0420750 1.0664610

H -1.0044760 0.8766570 0.1069560

H -4.1253800 -2.1606730 0.5065530

H -6.4365030 -1.1542290 0.5787440

H -4.9907970 2.5403720 -0.5415970

H -2.6696360 1.7165600 -0.6600140

**deZ optimized at CAM-B3LYP/cc-pVDZ**

Symbol X Y Z

C 3.1727620 0.4371250 0.7683850

C 2.2328530 -0.0584530 -0.2299800

C 1.6786610 0.8055910 -1.1873460

C 1.9636420 2.1652150 -1.2261700

C 2.8480040 2.6778410 -0.2570920

C 3.4222110 1.8624820 0.6901900

C 1.8982050 -1.5029180 -0.2509320

C 3.0235460 -2.4948610 -0.2637350

O 3.7172250 -0.2877380 1.6366750

N 0.7091900 -2.0058490 -0.2495090

N -0.3135420 -1.0909390 -0.1328470

C -1.6133190 -1.4611810 -0.1498350

O -2.0332100 -2.5975000 -0.3032630

C -2.5850250 -0.3123420 0.0326510

C -2.2726840 1.0419260 -0.0958970

C -3.2859560 1.9811320 0.0798250

N -4.5530910 1.6757990 0.3647070

C -4.8410420 0.3754710 0.4744670

C -3.9097010 -0.6418630 0.3134800

H 3.0889570 3.7467880 -0.2613890

H 1.5331060 2.8067400 -1.9971450

H 1.0116750 0.3815800 -1.9458700

H 4.1155970 2.2610850 1.4357270

H 3.6395520 -2.3588080 -1.1682340

H 3.6596960 -2.2790250 0.6067990

H 2.6278040 -3.5187200 -0.2324290

H -0.0508030 -0.1348260 0.1017130

H -4.1782270 -1.6949910 0.3917250

H -5.8843710 0.1337170 0.7033350

H -3.0582490 3.0472250 -0.0193160

H -1.2676890 1.3870820 -0.3467300

**deZ optimized at B3LYP/cc-pVDZ**

Symbol X Y Z

C 3.2448280 0.4222110 0.7478220

C 2.2557040 -0.0683610 -0.2239280

C 1.6818790 0.8130780 -1.1660860

C 1.9901840 2.1724610 -1.2158280

C 2.9157100 2.6776730 -0.2746520

C 3.5097170 1.8504850 0.6582110

C 1.8935960 -1.5056450 -0.2391790

C 2.9995720 -2.5279680 -0.2260360

O 3.8151700 -0.3040300 1.6047120

N 0.6889190 -2.0013180 -0.2515130

N -0.3342810 -1.0832340 -0.1421720

C -1.6428830 -1.4532740 -0.1633000

O -2.0614770 -2.5954130 -0.3310150

C -2.6160590 -0.3043920 0.0325930

C -2.3073780 1.0607790 -0.0685090

C -3.3274300 1.9988310 0.1155770

N -4.6037670 1.6882180 0.3854760

C -4.8883870 0.3785150 0.4697070

C -3.9507510 -0.6386230 0.2978790

H 3.1725200 3.7440710 -0.2908510

H 1.5476310 2.8184320 -1.9779650

H 0.9916060 0.4016740 -1.9115150

H 4.2348910 2.2402170 1.3795820

H 3.6395790 -2.4119700 -1.1191050

H 3.6295090 -2.3270090 0.6544070

H 2.5791830 -3.5436680 -0.2002240

H -0.0745150 -0.1244930 0.0942950

H -4.2212750 -1.6934820 0.3564250

H -5.9340530 0.1298780 0.6859120

H -3.0996870 3.0677690 0.0364610

H -1.3008480 1.4138310 -0.3051630

**deZ optimized at M062X/cc-pVDZ**

Symbol X Y Z

C 3.1693410 0.4601670 0.7520210

C 2.2142660 -0.0521090 -0.2243530

C 1.6101420 0.7992270 -1.1648350

C 1.8603990 2.1665840 -1.2088560

C 2.7633060 2.6975090 -0.2635370

C 3.3855770 1.8938280 0.6653550

C 1.9072480 -1.5027710 -0.2420500

C 3.0504430 -2.4753320 -0.2855030

O 3.7457100 -0.2518900 1.6067690

N 0.7244510 -2.0250690 -0.2295010

N -0.3032730 -1.1206450 -0.0932350

C -1.6027520 -1.4920220 -0.1372760

O -2.0264380 -2.6213540 -0.3138900

C -2.5641560 -0.3320290 0.0410320

C -2.2336380 1.0162130 -0.1170140

C -3.2370140 1.9707640 0.0519850

N -4.5064930 1.6858180 0.3551810

C -4.8087360 0.3895800 0.4903020

C -3.8904140 -0.6443830 0.3382150

H 2.9790620 3.7709120 -0.2717910

H 1.3920820 2.7986200 -1.9640010

H 0.9280580 0.3562610 -1.8996960

H 4.0895750 2.3090340 1.3906860

H 3.6506950 -2.3022780 -1.1927780

H 3.6930050 -2.2736330 0.5822660

H 2.6691430 -3.5041690 -0.2766650

H -0.0529820 -0.1698220 0.1762910

H -4.1714360 -1.6926010 0.4362780

H -5.8520960 0.1662510 0.7325480

H -2.9995550 3.0313880 -0.0690880

H -1.2265730 1.3439060 -0.3871130

**deZ optimized at PBE1PBE/cc-pVDZ**

Symbol X Y Z

C 3.1925710 0.4470520 0.7435720

C 2.2274020 -0.0627650 -0.2310020

C 1.6368400 0.7979780 -1.1747230

C 1.9029510 2.1626220 -1.2196760

C 2.8038220 2.6881230 -0.2721700

C 3.4144510 1.8774090 0.6595710

C 1.9001780 -1.5029140 -0.2436970

C 3.0231300 -2.4915520 -0.2371780

O 3.7755210 -0.2650220 1.5963500

N 0.7064150 -2.0130670 -0.2409300

N -0.3097600 -1.1073570 -0.1271560

C -1.6119670 -1.4719410 -0.1456090

O -2.0370120 -2.6084190 -0.3021900

C -2.5714510 -0.3189350 0.0385860

C -2.2519390 1.0386950 -0.0665040

C -3.2651920 1.9800660 0.1078140

N -4.5399680 1.6804370 0.3708490

C -4.8330280 0.3785000 0.4583670

C -3.9047190 -0.6435160 0.2966310

H 3.0297720 3.7608430 -0.2813430

H 1.4477530 2.7969430 -1.9831460

H 0.9630330 0.3643950 -1.9231330

H 4.1221480 2.2869800 1.3865000

H 3.6458900 -2.3681490 -1.1393720

H 3.6573600 -2.2591820 0.6327400

H 2.6287550 -3.5157680 -0.1920890

H -0.0460330 -0.1451790 0.0904670

H -4.1784540 -1.6976680 0.3567710

H -5.8813450 0.1386780 0.6695100

H -3.0304170 3.0468510 0.0258510

H -1.2416390 1.3857580 -0.2992730

**deE optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.8296000 0.9417820 -0.2478110

C 2.7938980 0.0125920 0.1206850

C 3.1055150 -1.3174890 0.4034030

C 4.3995320 -1.7965540 0.3814780

C 5.4266380 -0.9067380 0.0581680

C 5.1567680 0.4063660 -0.2362600

C 1.3914180 0.4459420 0.1922370

C 1.0561650 1.7916650 0.7722870

O 3.6006660 2.1440540 -0.5890210

N 0.4935410 -0.3926790 -0.1813830

N -0.8155450 -0.0165910 -0.0224960

C -1.8217520 -0.8577160 -0.3484740

O -1.6648300 -1.9910300 -0.7685550

C -3.1989090 -0.2963070 -0.1410670

C -3.5078730 1.0509940 -0.2484580

C -4.8200820 1.4498630 -0.0612150

N -5.8088680 0.6102600 0.2237170

C -5.5055640 -0.6817860 0.3192890

C -4.2296400 -1.1792610 0.1384780

H 6.4528550 -1.2551210 0.0416150

H 4.6122740 -2.8284690 0.6220020

H 2.2912590 -1.9810700 0.6634290

H 5.9579160 1.0876560 -0.4956700

H 1.9614210 2.3478700 0.9735850

H 0.4523790 2.3872530 0.0846860

H 0.4867810 1.6674960 1.6972840

H -1.0387430 0.8667960 0.4084190

H -4.0316760 -2.2375240 0.2122780

H -6.3227960 -1.3537730 0.5498220

H -5.0833290 2.4964340 -0.1502810

H -2.7632100 1.7912240 -0.5018750

**deZ optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.0042490 0.3921090 0.9245040

C 2.2523200 -0.0489110 -0.2171390

C 1.9112700 0.8298850 -1.2403400

C 2.2852280 2.1622460 -1.2169460

C 3.0242200 2.6170780 -0.1252020

C 3.3735270 1.7725280 0.9020750

C 1.8840750 -1.4808160 -0.3141570

C 2.9897230 -2.4820960 -0.4191290

O 3.3044400 -0.3816580 1.8858570

N 0.6904220 -1.9388330 -0.3377010

N -0.3242950 -1.0227200 -0.2072210

C -1.6149550 -1.4136880 -0.1868770

O -1.9884930 -2.5696130 -0.2909290

C -2.6062630 -0.2971310 -0.0168030

C -2.3694810 1.0148910 -0.3973630

C -3.3703290 1.9527720 -0.2119740

N -4.5539170 1.6681530 0.3193270

C -4.7756570 0.4061220 0.6772110

C -3.8449940 -0.6031510 0.5229740

H 3.3317750 3.6553910 -0.0839820

H 2.0179920 2.8260120 -2.0262970

H 1.3501330 0.4514460 -2.0875840

H 3.9476030 2.1413400 1.7433270

H 3.5471090 -2.3253040 -1.3442180

H 3.6772660 -2.3347970 0.4113250

H 2.5981940 -3.4963450 -0.4048380

H -0.0742840 -0.0599330 -0.0281400

H -4.0718120 -1.6168190 0.8152950

H -5.7456930 0.1892920 1.1069100

H -3.2077680 2.9808410 -0.5106280

H -1.4411640 1.3218350 -0.8564400

**E optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C -3.5510380 0.9943450 -0.4680410

C -3.1257540 -0.2505960 -0.0317200

C -4.0757230 -1.1346210 0.4536300

C -5.3962680 -0.7317640 0.5015500

N -5.8125020 0.4629340 0.0901690

C -4.8990000 1.2991630 -0.3887070

C -1.7010360 -0.7065800 -0.0872450

O -1.4073420 -1.8805400 -0.1931650

N -0.7747200 0.2878840 -0.0074610

N 0.5420400 -0.0398580 -0.0185620

C 1.4380840 0.8771710 0.0318850

C 1.0806570 2.3317140 0.0785030

C 2.8386860 0.4223160 0.0419940

C 3.8879770 1.3282950 0.2255030

C 5.2075610 0.9316770 0.2361540

C 5.5162810 -0.4098530 0.0557150

C 4.5095920 -1.3332740 -0.1191740

C 3.1739920 -0.9411210 -0.1195440

O 2.2562590 -1.9058540 -0.2808310

H 6.5470310 -0.7363190 0.0560000

H 5.9900460 1.6613230 0.3834010

H 3.6677010 2.3732900 0.3747740

H 4.7283520 -2.3829860 -0.2542150

H 1.3636770 -1.4822180 -0.2126390

H 1.9172910 2.9723030 -0.1661730

H 0.2891930 2.5494690 -0.6380290

H 0.7235350 2.6098250 1.0716050

H -1.0617710 1.2279520 0.2154190

H -3.7832410 -2.1179980 0.7881310

H -6.1545720 -1.4015370 0.8870070

H -5.2551760 2.2621880 -0.7321140

H -2.8712150 1.7179010 -0.8932420

**Z optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 2.4274060 -0.9850200 -0.5348040

C 2.6200600 0.2950090 -0.0393270

C 3.8188650 0.5753910 0.5960470

C 4.7558510 -0.4312660 0.7266460

N 4.5770010 -1.6635120 0.2579300

C 3.4326170 -1.9214090 -0.3642710

C 1.6215820 1.4053750 -0.1860990

O 1.9740880 2.5676350 -0.2318230

N 0.3292340 0.9979110 -0.2526980

N -0.6771690 1.9112320 -0.3924580

C -1.8760100 1.4834600 -0.3816140

C -2.9773790 2.4827750 -0.5200390

C -2.2565140 0.0472240 -0.2630500

C -2.1034060 -0.8220380 -1.3370270

C -2.4898730 -2.1476010 -1.2448460

C -3.0362060 -2.6149270 -0.0608970

C -3.1955650 -1.7674640 1.0201760

C -2.8086860 -0.4391840 0.9211000

O -2.9364660 0.4336510 1.9528130

H -3.3418110 -3.6480120 0.0258250

H -2.3674080 -2.8079850 -2.0905280

H -1.6817590 -0.4458020 -2.2594280

H -3.6183660 -2.1322870 1.9472270

H -3.3453180 0.0000600 2.7088470

H -3.5575200 2.2794610 -1.4211240

H -3.6584260 2.4068480 0.3271230

H -2.5731460 3.4899270 -0.5714900

H 0.0969470 0.0264890 -0.1011160

H 4.0110170 1.5652220 0.9804840

H 5.6948280 -0.2372050 1.2296840

H 3.3068630 -2.9243580 -0.7523720

H 1.5332210 -1.2640180 -1.0724460

**deE + 5H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 4.0493080 -0.9711190 -0.2665340

C 2.9624040 -0.0269500 -0.2219920

C 3.2370660 1.3466820 -0.1076180

C 4.5141810 1.8414180 -0.0659580

C 5.5847390 0.9363010 -0.1412810

C 5.3671520 -0.4056210 -0.2460110

C 1.5787380 -0.4709830 -0.2764860

C 1.2231010 -1.7562930 -0.9732470

O 3.8819530 -2.2284510 -0.2946510

N 0.6673570 0.2946700 0.2339930

N -0.6327150 -0.1406390 0.1233220

C -1.6663250 0.6655560 0.4142910

O -1.5638400 1.8364700 0.7515610

C -3.0110210 0.0217860 0.2555980

C -3.2938800 -1.2500890 0.7294760

C -4.5679450 -1.7575600 0.5524850

N -5.5358010 -1.0868640 -0.0601680

C -5.2583630 0.1330750 -0.5125680

C -4.0220520 0.7325250 -0.3745510

H 6.6022430 1.3096500 -0.1210050

H 4.6899130 2.9053780 0.0037590

H 2.4036250 2.0335660 -0.0581800

H 6.1886600 -1.1073500 -0.3002190

H 2.1052140 -2.2026790 -1.4116400

H 0.8272310 -2.4919160 -0.2681560

H 0.4666650 -1.5674860 -1.7399530

H -0.8222710 -1.0696760 -0.2174360

H -3.8352050 1.7262330 -0.7606390

H -6.0664260 0.6551590 -1.0090690

H -4.8321260 -2.7415340 0.9200470

H -2.5485420 -1.8312500 1.2537220

H 5.2536590 -3.2346550 -0.2893830

O 6.0721410 -3.7790830 -0.1720770

H 6.2118690 -3.7561820 0.7763500

H -7.0579480 -2.2385190 -0.0642160

O -7.6416840 -3.0190350 -0.0276870

H -7.4722120 -3.4788300 -0.8521350

H -0.2456940 2.8366080 -0.2094520

O 0.0456410 3.3615580 -0.9743310

H 0.7157240 2.8180630 -1.3946560

H 1.1272920 1.3487890 1.9546200

O 1.5853000 1.6966600 2.7341720

H 2.5120430 1.6006020 2.5007180

H -2.6717720 3.4685580 -0.1186670

O -2.7964720 3.8217480 -1.0067080

H -1.8907710 3.7959850 -1.3502930

**deZ + 5H2O optimized at CAM-B3LYP/cc-pVTZ**

Tag Symbol X Y Z

C -2.0638950 -0.9536260 0.7785370

C -2.9075980 -0.2020510 -0.0893880

C -4.0271250 -0.8218640 -0.6535790

C -4.3183200 -2.1517080 -0.4479470

C -3.4757010 -2.8998760 0.3709650

C -2.3806960 -2.3219230 0.9659020

C -2.6720820 1.2318780 -0.3839470

C -3.8612980 2.1534580 -0.3676330

O -1.0314450 -0.4320230 1.3660360

N -1.5629270 1.8046250 0.6668340

N -0.4317030 1.0210880 -0.7050610

C 0.7462250 1.6284930 -1.0085640

O 0.8732750 2.7615070 -1.4295030

C 1.9485250 0.7578180 -0.7682430

C 1.9665020 -0.6049060 -1.0262870

C 3.1386940 -1.3019540 -0.7938390

N 4.2444340 -0.7379620 -0.3213220

C 4.2132240 0.5663250 -0.0635080

C 3.1005120 1.3537800 -0.2783800

H -3.6825530 -3.9487070 0.5440950

H -5.1781120 -2.6043480 -0.9205930

H -4.6738220 -0.2430990 -1.2986590

H -1.7171870 -2.8936720 1.6001720

H -4.5995690 1.8683510 -1.1170610

H -4.3594480 2.1178960 0.6017940

H -3.5335960 3.1682860 -0.5735640

H -0.4075650 0.2869470 0.0329030

H 3.1018210 2.4051760 -0.0335070

H 5.1230190 0.9976420 0.3350410

H 3.1970610 -2.3639450 -0.9998600

H 1.0997420 -1.1255540 -1.4100670

H 5.6222490 -1.9978190 -0.0600250

O 6.1966720 -2.7673200 0.1235310

H 5.9046930 -3.0713750 0.9851460

H 0.0810510 -1.5766570 2.1404320

O 0.6959230 -2.2833670 2.4310690

H 1.3217590 -2.3555830 1.7078130

H 1.1873260 3.8460680 0.3548430

O 1.4645020 3.9130190 1.2759540

H 0.8736390 3.3013410 1.7447230

H -1.1556050 -1.1624680 -2.1706250

O -0.8990160 -2.0897520 -2.1842320

H -1.3625760 -2.4568030 -1.4224670

H -1.1897060 2.6291490 1.5461620

O -0.6823420 2.2337510 2.2621700

H -0.7836050 1.2753300 2.1010910

**E + 5H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.2101060 0.1895320 0.3032930

C 2.2797820 -0.7337800 -0.1401860

C 2.7183390 -1.9996790 -0.5058540

C 4.0657990 -2.2877760 -0.4019910

N 4.9612280 -1.4078930 0.0338490

C 4.5365390 -0.1962580 0.3755240

C 0.8530900 -0.3080030 -0.2232360

O 0.5197240 0.8399020 -0.4142930

N -0.0699540 -1.3092810 -0.0594010

N -1.3767660 -0.9565870 -0.0481110

C -2.3235580 -1.8054400 0.0912970

C -2.0997150 -3.2828230 0.2271260

C -3.6879330 -1.2553150 0.1227650

C -3.9370770 0.1217980 -0.0625040

C -5.2403220 0.6034870 -0.0299970

C -6.2981270 -0.2478320 0.1957830

C -6.0750860 -1.6028920 0.3962160

C -4.7868070 -2.0866730 0.3568860

O -2.9565180 1.0152440 -0.2762660

O -2.3041940 3.7741290 -0.2755290

O 2.4032010 4.9216400 0.1342660

O 7.1204750 -3.2670720 -0.3050060

O 3.9312810 3.0294500 1.3730000

O 0.3929170 3.6255360 -1.0694650

H -7.3045520 0.1462070 0.2181810

H -6.9006480 -2.2740890 0.5807480

H -4.6275280 -3.1415260 0.5209200

H -5.3932970 1.6616550 -0.1864080

H -2.8587460 -3.8388910 -0.3147660

H -1.1368420 -3.5855810 -0.1765840

H -2.1470170 -3.5907880 1.2724530

H 0.2254870 -2.2148850 0.2675270

H 2.9367870 1.1906370 0.6029030

H 5.2778380 0.5124440 0.7196660

H 4.4569460 -3.2568370 -0.6853540

H 2.0456090 -2.7455760 -0.9053220

H -2.6482490 2.8689200 -0.3287730

H -2.2902630 3.9847230 0.6610630

H 6.5999770 -2.4611510 -0.1484240

H 7.3714310 -3.5706410 0.5694630

H 2.8158390 5.4068440 -0.5828340

H 1.6157480 4.4841720 -0.2677300

H 0.5480520 2.6794510 -0.9536100

H -0.5467010 3.7578390 -0.8509200

H 3.8660200 3.2806540 2.2961700

H 3.4351040 3.7258960 0.8921180

H -2.0878220 0.5361360 -0.2492240

**Z + 5H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.2981580 0.9529560 -0.2777350

C 2.1495520 0.3195790 -0.7298330

C 2.2323740 -1.0196510 -1.0723620

C 3.4488370 -1.6641090 -0.9299680

N 4.5441570 -1.0631860 -0.4863360

C 4.4655790 0.2259170 -0.1687160

C 0.9131470 1.1498450 -0.8709110

O 0.9891040 2.3718350 -0.8261840

N -0.2669040 0.5056000 -1.0467690

N -1.3052100 1.2650820 -1.5209490

C -2.5055950 0.8774420 -1.3722670

C -3.5738430 1.7220440 -1.9946730

C -2.9546590 -0.3179690 -0.6117630

C -2.9809890 -0.3056150 0.7825150

C -3.4746340 -1.4066550 1.4725620

C -3.9186190 -2.5190820 0.7876490

C -3.8867470 -2.5479860 -0.5990200

C -3.4196740 -1.4432070 -1.2835190

O -2.5416250 0.7290280 1.5389130

O -0.1559280 -0.6262900 2.5770160

O 7.3380640 -1.2892500 0.1507300

O 1.0678740 1.8614500 2.6005670

O -0.9469250 2.9457430 0.9276120

O -0.2812760 -2.0541910 0.2608260

H -4.2936620 -3.3691630 1.3401230

H -4.2334940 -3.4167410 -1.1388720

H -3.4032070 -1.4480190 -2.3653260

H -3.4937980 -1.3700670 2.5523090

H -4.1513250 1.1370010 -2.7119600

H -4.2761360 2.0667620 -1.2340910

H -3.1313580 2.5747900 -2.5013210

H -0.3902490 -0.4674840 -0.7360370

H 3.2708090 2.0055560 0.0408780

H 5.3838840 0.6820170 0.1787250

H 3.5429970 -2.7114090 -1.1862630

H 1.3783510 -1.5722340 -1.4254600

H 6.4285880 -1.4410030 -0.1567730

H 7.3605230 -1.6561600 1.0366660

H -1.0213200 -0.1987960 2.5554310

H 0.4603620 0.1266280 2.6416990

H 1.9088020 2.0916690 2.2001320

H 0.3935840 2.3645740 2.1125520

H -1.0957490 -2.5600880 0.3227830

H -0.1591090 -1.6365710 1.1443320

H -0.3750680 2.9231490 0.1242980

H -1.3252300 3.8260440 0.9843770

H -2.0941490 1.4494250 1.0543460

**Structure 1 - deE + H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.5054780 0.3356080 0.0636470

C 2.3585190 -0.5256120 0.1598800

C 2.5256380 -1.9150350 0.1640980

C 3.7642280 -2.5086380 0.1177880

C 4.8942920 -1.6852160 0.0593650

C 4.7751760 -0.3228340 0.0401840

C 1.0014520 0.0164710 0.2386190

C 0.7693680 1.3694100 0.8611420

O 3.4232110 1.6050290 -0.0199120

N 0.0294040 -0.7225570 -0.1719510

N -1.2317570 -0.2034600 -0.0284530

C -2.3383720 -0.9244820 -0.3116220

O -2.3620530 -2.0875030 -0.6573120

C -3.6283720 -0.1581530 -0.1450250

C -3.7522250 1.2198310 -0.2455840

C -5.0026350 1.7944190 -0.0950490

N -6.1084330 1.1021510 0.1458490

C -5.9840010 -0.2191620 0.2305990

C -4.7840800 -0.8872000 0.0861570

H 5.8825360 -2.1316200 0.0321880

H 3.8615650 -3.5854390 0.1372000

H 1.6328140 -2.5231770 0.2154960

H 5.6466940 0.3165400 -0.0107290

H 1.7108570 1.8038810 1.1705970

H 0.3277340 2.0662730 0.1435230

H 0.0910060 1.2781230 1.7152680

H -1.3455490 0.7202310 0.3557240

H -4.7227710 -1.9638230 0.1390290

H -6.8960330 -0.7728390 0.4218170

H -5.1175930 2.8690240 -0.1786370

H -2.9039470 1.8511670 -0.4687980

H 4.8267460 2.4980120 -0.2188490

O 5.6625360 2.9842990 -0.4517800

H 5.7651050 2.7896650 -1.3851090

**Structure 2 - deE + H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C -3.7916430 -1.2283350 0.3414540

C -2.7483050 -0.3154040 -0.0863770

C -3.0873990 0.9651030 -0.5557030

C -4.3825800 1.4021390 -0.6531330

C -5.4125150 0.5277060 -0.2667190

C -5.1344770 -0.7225250 0.1970490

C -1.3431300 -0.6827140 -0.0326350

C -0.9452450 -2.1361980 -0.0670650

O -3.5928050 -2.3699660 0.8284530

N -0.4569340 0.2619530 -0.0168570

N 0.8549360 -0.1446690 -0.0434550

C 1.8718570 0.7313720 -0.0799950

O 1.7657990 1.9473140 -0.1156790

C 3.2405930 0.1042350 -0.0644980

C 3.5267260 -1.1861600 -0.4867670

C 4.8351620 -1.6338860 -0.4366800

N 5.8507350 -0.8981480 -0.0032790

C 5.5708430 0.3407440 0.3898840

C 4.3007960 0.8832530 0.3713200

H -6.4453620 0.8515510 -0.3424390

H -4.6044240 2.3897070 -1.0325350

H -2.2814460 1.6177710 -0.8636680

H -5.9232900 -1.3987700 0.5010360

H -1.8338140 -2.7560130 -0.0826960

H -0.3161230 -2.3296600 -0.9414220

H -0.3843150 -2.4181040 0.8290570

H 1.0678830 -1.1202980 0.0870400

H 4.1129830 1.9004470 0.6802300

H 6.4100410 0.9325300 0.7366230

H 5.0764430 -2.6369180 -0.7692830

H 2.7609340 -1.8389860 -0.8809760

H 0.1961320 2.9759560 0.2607240

O -0.5933010 3.4552810 0.5552640

H -1.2184470 2.7398200 0.6983340

**Structure 3 - deE + H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 3.7907630 -1.2623640 0.1709740

C 2.7441120 -0.3056580 -0.1353770

C 3.0786660 1.0185490 -0.4639420

C 4.3738670 1.4624720 -0.5314810

C 5.4065870 0.5493840 -0.2601980

C 5.1323510 -0.7450990 0.0647100

C 1.3393030 -0.6770060 -0.1000010

C 0.9393300 -2.1129980 -0.3255740

O 3.5938250 -2.4511280 0.5294180

N 0.4567420 0.2559350 0.0673140

N -0.8563500 -0.1424940 0.0101980

C -1.8723420 0.7332030 0.0694440

O -1.7655860 1.9470150 0.1493190

C -3.2404310 0.1081350 0.0083770

C -3.5332470 -1.1940670 0.3875260

C -4.8399330 -1.6409600 0.2982600

N -5.8473530 -0.8938100 -0.1346700

C -5.5613180 0.3564110 -0.4854080

C -4.2927250 0.8991210 -0.4251370

H 6.4390930 0.8785900 -0.3146660

H 4.5927940 2.4856430 -0.8028110

H 2.2701270 1.7018900 -0.6870020

H 5.9240570 -1.4515810 0.2793180

H 1.8282440 -2.7263240 -0.4141260

H 0.3686340 -2.5046120 0.5214000

H 0.3203800 -2.1945330 -1.2249070

H -1.0674070 -1.1125650 -0.1581800

H -4.1006120 1.9255890 -0.6987370

H -6.3942910 0.9575720 -0.8310760

H -5.0867390 -2.6531020 0.5974750

H -2.7743700 -1.8564390 0.7791210

H 1.2378420 2.6833600 0.9505000

O 0.6172000 3.4096780 0.8487490

H -0.1824210 2.9498310 0.5508670

**Structure 4 - deE + H2O optimized at CAM-B3LYP/cc-pVTZ**

Symbol X Y Z

C 4.3457130 1.1809460 -0.0678040

C 3.3567900 0.1250080 0.0469090

C 3.7715920 -1.2156410 0.0994530

C 5.0899780 -1.5909030 0.0777460

C 6.0672760 -0.5854380 -0.0050580

C 5.7154110 0.7294060 -0.0669050

C 1.9272540 0.4021530 0.0964500

C 1.4387770 1.7710840 0.4984820

O 4.0871870 2.4067590 -0.1837100

N 1.1036800 -0.5633970 -0.1566220

N -0.2293490 -0.2649870 -0.0429490

C -1.1869610 -1.2011660 -0.1877430

O -1.0095070 -2.3867130 -0.3884300

C -2.5941300 -0.6660990 -0.0649250

C -2.9730210 0.6487380 -0.2978810

C -4.3059710 0.9956700 -0.1797530

N -5.2580850 0.1312240 0.1514010

C -4.8956700 -1.1307400 0.3666270

C -3.5928390 -1.5708020 0.2633930

H 7.1176380 -0.8583210 -0.0168350

H 5.3693850 -2.6341010 0.1341130

H 2.9981280 -1.9682050 0.1690600

H 6.4628690 1.5094630 -0.1370920

H 2.2890760 2.4254210 0.6557520

H 0.8306320 2.2220570 -0.2915110

H 0.8274530 1.7037150 1.4040790

H -0.5035240 0.6650840 0.2290450

H -3.3278630 -2.6054720 0.4198340

H -5.6904080 -1.8175330 0.6308160

H -4.6313690 2.0126220 -0.3624550

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H -6.9322710 1.0125410 0.1500340

O -7.6980060 1.5998120 -0.0011200

H -7.8876800 1.4999580 -0.9358960