## Table S1

Geometry parameters of the precursor complex P1 optimized at different theory levels without symmetry constraints. All the distances are given in Å. For comparison we have also given some experimental (EXAFS) and calculated bond distances for other uranyl(VI) complexes containing fluoride[17].

| ***Distance between atoms*** | ***SCF optimised geometry*** | ***RI-MP2 optimised geometry*** |
|---|---|---|
| $U_A$-$U_B$ | 6.616 | 6.581 |
| $U_A$-F | 2.300 | 2.261 |
| $U_A$-$O_{yl}$ | 1.719, 1.719 | 1.784, 1.784 |
| $U_A$-$O_{water}$ | 2.495, 2.506, 2.507, 2.498 | 2.495, 2.509, 2.489, 2.477, |
| $U_B$-F | 4.316 | 4.327 |
| $U_B$-$O_{yl}$ | 1.715, 1.715 | 1.779, 1.779 |
| $U_B$-$O_{water}$ | 2.476[a], 2.495, 2.480, 2.495, 2.475[a] | 2.465[a], 2.477, 2.462, 2.478, 2.466[a] |
| F – H | 1.719, 1.719 | 1.676, 1.676 |
| U – F and U – $OH_2$ distances in $UO_2F(OH_2)_4^+$ from Gaillard *et al*.[18] | | |
| U- F (EXAFS)<br>U- $OH_2$ (EXAFS) | 2.24 ± 0.02<br>2.42 ± 0.02 | |
| U – F bond distances in $UO_2(oxalate)_2F^{3-}$, from ref. 17 | | |
| U – F (EXAFS) | 2.22 ± 0.02 | |
| U – F | 2.21 (SCF, gas phase) | 2.22(SCF, CPCM) |
| $UO_2F_4(OH_2)^{2-}$, from ref. 17 | | |
| U – F (EXAFS)<br>U – $OH_2$ (EXAFS) | 2.26 ± 0.02<br>2.48 ± 0.02 | |
| U – F<br>U – $OH_2$ | 2.28 ± 0.04 (SCF, gas phase)<br>2.75 (SCF, gas phase) | 2.28 ± 0.04 (SCF, CPCM)<br>2.62 (SCF, CPCM) |

[a] – distance to the oxygen atom in the water molecule that is a hydrogen bond donor

## Coordinates of all complexes

## Total water molecules 9

***Precursor geometry***

SCF-optimised without symmetry constraints

E(SCF,small basis,gas phase)=-1189.35308176

| | | | |
|---|---|---|---|
| U | -0.008804 | 0.000525 | -3.284680 |
| U | 0.002134 | 0.002061 | 3.330940 |
| F | 0.005284 | 0.006374 | -0.984829 |
| O | -2.408287 | 0.147353 | -2.616858 |
| O | 2.389711 | -0.165633 | -2.607545 |
| O | 0.145612 | 1.712597 | -3.304702 |
| O | -0.171454 | -1.710809 | -3.309608 |
| O | -1.435101 | 0.177332 | -5.337423 |

| | | | |
|---|---|---|---|
| O | 1.452113 | -0.172735 | -5.314879 |
| O | -1.705083 | -0.151897 | 3.390805 |
| O | 1.709582 | 0.155967 | 3.385419 |
| O | -0.209344 | 2.406251 | 3.965059 |
| O | 0.214164 | -2.403269 | 3.960488 |
| O | -0.127190 | 1.385512 | 1.281989 |
| O | 0.127030 | -1.377831 | 1.279523 |
| O | 0.006465 | 0.000159 | 5.810588 |
| H | -1.396911 | 0.900104 | -5.954675 |
| H | -2.073168 | -0.470529 | -5.615966 |
| H | 2.094055 | 0.477136 | -5.579703 |
| H | 1.409409 | -0.882458 | -5.946789 |
| H | -2.970352 | 0.896476 | -2.779092 |
| H | -2.880532 | -0.542284 | -2.165262 |
| H | 2.836428 | 0.471605 | -2.063147 |
| H | 2.971832 | -0.876294 | -2.850984 |
| H | -1.032083 | 2.832426 | 4.184533 |
| H | -0.522209 | -2.965967 | 4.179281 |
| H | 0.527258 | 2.969409 | 4.181891 |
| H | 1.037286 | -2.830720 | 4.175998 |
| H | -0.205138 | 2.329684 | 1.304092 |
| H | 0.201633 | -2.322314 | 1.299828 |
| H | -0.105455 | 1.044458 | 0.380454 |
| H | 0.106195 | -1.035143 | 0.378583 |
| H | -0.771124 | -0.070825 | 6.355207 |
| H | 0.786039 | 0.070315 | 6.352472 |

DFT-optimized without symmetry constraints
E(b3lyp,small basis, gas phase)=-1197.31552756
**(Complex P2)**

| | | | |
|---|---|---|---|
| U | -0.011094 | 0.001593 | -3.263479 |
| U | 0.002018 | 0.001567 | 3.324358 |
| F | 0.008886 | 0.010129 | -0.973433 |
| O | -2.393031 | 0.080428 | -2.600259 |
| O | 2.376581 | -0.082793 | -2.602119 |
| O | 0.131342 | 1.772316 | -3.294383 |
| O | -0.172511 | -1.767636 | -3.294800 |
| O | -1.419508 | 0.238975 | -5.299275 |
| O | 1.441846 | -0.252143 | -5.271536 |
| O | -1.762692 | -0.139965 | 3.429907 |
| O | 1.766867 | 0.143069 | 3.427980 |
| O | -0.184141 | 2.399022 | 3.916273 |
| O | 0.188065 | -2.397859 | 3.908025 |
| O | -0.110402 | 1.365601 | 1.282244 |
| O | 0.113758 | -1.354689 | 1.277403 |
| O | 0.003319 | -0.002566 | 5.779758 |
| H | -1.398582 | 1.015733 | -5.883388 |
| H | -2.040613 | -0.425318 | -5.641691 |
| H | 2.081733 | 0.404548 | -5.593290 |
| H | 1.393462 | -1.006366 | -5.882650 |
| H | -2.975829 | 0.849236 | -2.712608 |
| H | -2.881337 | -0.668059 | -2.220879 |
| H | 2.840292 | 0.619979 | -2.119355 |
| H | 2.979386 | -0.815870 | -2.807551 |
| H | -1.018304 | 2.839425 | 4.155414 |
| H | -0.568954 | -2.960599 | 4.147291 |
| H | 0.573211 | 2.961608 | 4.154848 |
| H | 1.022663 | -2.840031 | 4.142343 |
| H | -0.183719 | 2.330686 | 1.315834 |
| H | 0.182893 | -2.320193 | 1.307571 |
| H | -0.090891 | 1.024819 | 0.351938 |
| H | 0.098039 | -1.010533 | 0.348259 |

| | | | |
|---|---|---|---|
| H | -0.791880 | -0.065890 | 6.336450 |
| H | 0.799121 | 0.058814 | 6.335808 |

RI-MP2 optimized without symmetry constraints.
E(RI-MP2, large basis, no ECP on O, gas phase)= -2036.0711410153

| | | | |
|---|---|---|---|
| U | -0.0142971 | -0.0051617 | -3.2678123 |
| U | 0.0008794 | -0.0030902 | 3.3131172 |
| F | 0.0484544 | 0.1218944 | -1.0113131 |
| O | -2.0206074 | -1.2929515 | -2.5939457 |
| O | 1.9591674 | 1.3378557 | -2.5405618 |
| O | -1.0478624 | 1.4420596 | -3.4054408 |
| O | 0.9038781 | -1.5345594 | -3.2787374 |
| O | -1.0936777 | -0.7829191 | -5.3717849 |
| O | 1.4180293 | 0.8130208 | -5.1583153 |
| O | -1.4107296 | -1.0808848 | 3.4158114 |
| O | 1.4138673 | 1.0713201 | 3.4325945 |
| O | -1.4599256 | 1.9000411 | 3.9313323 |
| O | 1.4596011 | -1.9309407 | 3.8535725 |
| O | -0.8231881 | 1.1083121 | 1.2719461 |
| O | 0.8140536 | -1.0367144 | 1.2278734 |
| O | 0.0169840 | -0.0405081 | 5.7743033 |
| H | -1.7720781 | -0.3167189 | -5.8856385 |
| H | -0.9236137 | -1.6115717 | -5.8471336 |
| H | 1.1766996 | 1.5358990 | -5.7599887 |
| H | 2.0287031 | 0.2494262 | -5.6606649 |
| H | -2.9351852 | -0.9718553 | -2.6233230 |
| H | -2.0796552 | -2.2595598 | -2.5437185 |
| H | 2.1101795 | 1.6924220 | -1.6540602 |
| H | 2.5878755 | 1.7750445 | -3.1330831 |
| H | -2.3725238 | 1.8217082 | 4.2560238 |
| H | 1.1461836 | -2.8027862 | 4.1469453 |
| H | -1.1467523 | 2.7684800 | 4.2350184 |
| H | 2.3812569 | -1.8678868 | 4.1552649 |
| H | -1.4458809 | 1.8480604 | 1.2616942 |
| H | 1.3922296 | -1.8106013 | 1.1842601 |
| H | -0.6114727 | 0.8676869 | 0.3387938 |
| H | 0.6196748 | -0.7420822 | 0.3063544 |
| H | -0.5939262 | -0.5212637 | 6.3570271 |
| H | 0.6366044 | 0.4232799 | 6.3616094 |

***Associative-Intermediate geometry***
SCF optimized (in PCM) without symmetry constraints.
The convergence threshold on the gradient norm was set to 0.002 a.u.
E(SCF, small basis, PCM)= -1189.88506997

| | | | |
|---|---|---|---|
| U | -1.858355 | -0.169664 | -0.082962 |
| U | 2.755035 | -0.106670 | 0.089850 |
| F | 0.485226 | -0.446703 | -0.198509 |
| O | -2.096261 | -1.615084 | -1.002728 |
| O | -1.376937 | 1.330985 | 0.660569 |
| O | -1.044323 | 0.715980 | -2.209702 |
| O | -3.591053 | 1.289308 | -1.060983 |
| O | -4.308165 | -1.018680 | 0.181488 |
| O | -2.995904 | 0.079710 | 2.248091 |
| O | -1.083757 | -1.748957 | 1.644918 |
| O | 2.849291 | 0.805896 | -1.376817 |
| O | 2.734929 | -1.008395 | 1.566109 |
| O | 2.408695 | -2.162793 | -1.217000 |
| O | 4.915544 | -1.103236 | -0.415714 |
| O | 4.326747 | 1.450783 | 1.100358 |
| O | 1.503525 | 1.735662 | 1.156686 |
| H | -1.130392 | 0.243065 | -3.038578 |

| | | | |
|---|---|---|---|
| H | -0.614760 | 1.562189 | -2.340047 |
| H | -4.467498 | 1.001336 | -1.310521 |
| H | -3.442780 | 2.203405 | -1.302192 |
| H | -4.571018 | -1.814006 | -0.278809 |
| H | -5.028385 | -0.659697 | 0.695508 |
| H | -3.624947 | -0.488164 | 2.690083 |
| H | -2.812992 | 0.864575 | 2.761928 |
| H | -0.561678 | -2.532411 | 1.474654 |
| H | -1.238865 | -1.633689 | 2.579767 |
| H | 1.572288 | -2.433086 | -1.595028 |
| H | 3.100032 | -2.788551 | -1.433511 |
| H | 5.431159 | -0.911225 | -1.202474 |
| H | 5.403765 | -1.676267 | 0.179860 |
| H | 4.741824 | 2.181520 | 0.636304 |
| H | 4.680471 | 1.367571 | 1.988799 |
| H | 1.913549 | 2.457279 | 1.633302 |
| H | 0.555208 | 1.826098 | 1.138838 |

DFT optimized without symmetry constraints
E(B3LYP,small basis,gas)= -1197.29747577
**(COMPLEX B2)**

| | | | |
|---|---|---|---|
| U | 2.431426 | -0.000399 | 0.007605 |
| U | -2.203935 | -0.064653 | -0.036688 |
| F | 0.130893 | -0.339841 | -0.007822 |
| O | 2.218460 | -2.450927 | -0.063929 |
| O | 1.175673 | 2.122978 | 0.024911 |
| O | 2.510246 | -0.005957 | -1.767048 |
| O | 2.485875 | -0.090740 | 1.781018 |
| O | 4.738982 | -0.871218 | -0.014328 |
| O | 3.938386 | 1.985265 | 0.106093 |
| O | -2.382461 | -1.831040 | -0.176662 |
| O | -1.644331 | 1.652037 | -0.056458 |
| O | -3.801112 | 1.115151 | -1.591102 |
| O | -3.435776 | 1.222284 | 1.812114 |
| O | -1.534272 | -0.455057 | -2.371817 |
| O | -1.591854 | -0.809950 | 2.240052 |
| O | -4.658731 | -0.760951 | 0.301149 |
| H | 5.242313 | -1.088653 | -0.817632 |
| H | 5.275353 | -1.054663 | 0.775961 |
| H | 4.407988 | 2.355422 | -0.661566 |
| H | 4.312425 | 2.342561 | 0.930312 |
| H | 2.177689 | -2.977810 | -0.879436 |
| H | 2.262098 | -3.033216 | 0.712831 |
| H | 1.589778 | 2.998966 | 0.032302 |
| H | 0.199162 | 2.177162 | 0.002275 |
| H | -4.504852 | 0.715301 | -2.128435 |
| H | -4.078552 | 0.879584 | 2.454536 |
| H | -3.755898 | 2.073708 | -1.743520 |
| H | -3.336031 | 2.184642 | 1.901098 |
| H | -1.453445 | -1.356826 | -2.723809 |
| H | -1.452683 | -1.748615 | 2.446152 |
| H | -1.356565 | 0.202114 | -3.064057 |
| H | -1.456230 | -0.256889 | 3.026106 |
| H | -4.864388 | -1.711434 | 0.293373 |
| H | -5.468097 | -0.232997 | 0.397641 |

RI-MP2 optimized without symmetry constraints
E(RI-MP2, large basis, no ECP on O, gas phase)= -2036.0585645754

| | | | |
|---|---|---|---|
| U | 2.1995964 | -0.0275805 | 0.0619314 |
| U | -2.3859432 | -0.0107235 | -0.0224121 |
| F | -0.0996953 | -0.2856982 | -0.0849886 |
| O | 2.2532505 | -1.7981018 | 0.2800783 |

| | | | |
|---|---|---|---|
| O | 1.7466397 | 1.7097348 | 0.2027495 |
| O | 1.3860310 | -0.1620370 | 2.3884834 |
| O | 4.1048512 | 0.5980991 | 1.5224214 |
| O | 4.5661666 | -1.0214640 | -0.6913875 |
| O | 3.5577920 | 1.3849760 | -1.7068598 |
| O | 1.6698583 | -0.5089501 | -2.3090130 |
| O | -2.4203925 | -0.0771383 | 1.7582691 |
| O | -2.5092604 | -0.0454296 | -1.7991511 |
| O | -2.0983355 | -2.4631479 | -0.0441820 |
| O | -4.6749252 | -0.9542933 | 0.0124165 |
| O | -3.9451271 | 1.9388203 | 0.0071602 |
| O | -1.2080855 | 2.1822271 | -0.0013819 |
| H | 1.4365990 | -0.9666101 | 2.9286351 |
| H | 1.1845560 | 0.5617747 | 3.0010014 |
| H | 4.8732554 | 0.0264728 | 1.6750664 |
| H | 4.2349160 | 1.3853736 | 2.0737014 |
| H | 4.6410991 | -1.9871873 | -0.7460947 |
| H | 5.4357312 | -0.6902924 | -0.9602412 |
| H | 4.3004370 | 1.1665987 | -2.2888514 |
| H | 3.5699077 | 2.3519117 | -1.6323563 |
| H | 1.3106965 | -1.3191796 | -2.7002222 |
| H | 1.8748970 | 0.0922578 | -3.0408944 |
| H | -2.0796365 | -3.0421415 | 0.7343572 |
| H | -2.2293216 | -3.0498260 | -0.8059823 |
| H | -5.1891298 | -1.2146790 | 0.7940095 |
| H | -5.2358507 | -1.1589070 | -0.7534530 |
| H | -4.4465815 | 2.2324611 | 0.7859124 |
| H | -4.4629257 | 2.2342496 | -0.7602083 |
| H | -1.6329230 | 3.0520541 | -0.0169268 |
| H | -0.2479810 | 2.3228061 | 0.0200451 |

***Associative-Transition State geometry 1***

B3LYP optimized without symmetry constraints

E(B3LYP, small basis, gas)= -1197.29248419

**(COMPLEX TB2)**

| | | | |
|---|---|---|---|
| U | -2.420168 | 0.010944 | -0.056493 |
| U | 2.289377 | 0.037915 | 0.058954 |
| F | -0.222950 | 0.633445 | -0.171795 |
| O | -2.406031 | 2.257264 | 0.968990 |
| O | -1.177111 | -1.436385 | -1.587112 |
| O | -3.060126 | 0.935235 | -1.428495 |
| O | -1.874760 | -0.889424 | 1.400234 |
| O | -4.567141 | 0.217434 | 1.141889 |
| O | -3.862248 | -1.821117 | -0.911384 |
| O | 3.036906 | 1.090605 | 1.271716 |
| O | 1.562223 | -1.064815 | -1.159016 |
| O | 3.692385 | 0.777977 | -1.842048 |
| O | 2.716187 | -2.286725 | 0.926443 |
| O | 1.619856 | 2.206542 | -0.900987 |
| O | 0.939518 | -0.359975 | 2.089775 |
| O | 4.777115 | -0.582044 | 0.128960 |
| H | -5.353072 | 0.694237 | 0.823526 |
| H | -4.752650 | -0.189168 | 2.005826 |
| H | -4.507529 | -1.685102 | -1.627477 |
| H | -3.994116 | -2.694959 | -0.504590 |
| H | -2.758135 | 3.026033 | 0.488036 |
| H | -2.170521 | 2.508659 | 1.877401 |
| H | -1.569339 | -2.029369 | -2.245997 |
| H | -0.200661 | -1.393808 | -1.661850 |
| H | 4.643258 | 0.585845 | -1.856197 |
| H | 3.042184 | -2.549324 | 1.803296 |
| H | 3.386562 | 1.144084 | -2.687127 |

| | | | |
|---|---|---|---|
| H | 2.462977 | -3.068435 | 0.408358 |
| H | 2.145752 | 3.021950 | -0.934691 |
| H | 1.210185 | -0.016103 | 2.956604 |
| H | 0.673616 | 2.361736 | -1.044205 |
| H | 0.054426 | -0.772141 | 2.123256 |
| H | 5.374759 | -0.055304 | 0.688086 |
| H | 5.177470 | -1.441445 | -0.084204 |

***Intermediate following a dissociation of water from A-intermediate***

SCF-optimised without symmetry constraints.

E(SCF,small basis,gas phase)=-1189. 35461249

| | | | |
|---|---|---|---|
| O | 2.572837 | -1.208611 | -1.05659 |
| U | 2.116353 | 0.074462 | -0.016702 |
| O | 1.125237 | -1.625873 | 1.52424 |
| F | -0.206395 | -0.056737 | -0.376704 |
| U | -2.518995 | -0.071054 | -0.055633 |
| O | -1.419317 | 1.755525 | 1.24701 |
| O | 1.624905 | 1.385670 | 1.00188 |
| O | 1.776112 | 1.466905 | -2.03843 |
| O | 4.286056 | 1.115536 | -0.533132 |
| O | 3.814327 | -0.682404 | 1.59500 |
| O | -2.879629 | 1.018096 | -1.32917 |
| O | -2.194567 | -1.201901 | 1.20819 |
| O | -2.122949 | -1.743650 | -1.83669 |
| O | -4.692500 | -1.217062 | -0.403324 |
| O | -4.177366 | 1.147108 | 1.36231 |
| O | 6.199322 | -0.738130 | 0.230525 |
| H | 2.103745 | 1.201176 | -2.89203 |
| H | 1.325687 | 2.302302 | -2.09704 |
| H | 5.096517 | 0.604079 | -0.433912 |
| H | 4.462793 | 2.019074 | -0.763883 |
| H | 6.410217 | -1.457183 | -0.355655 |
| H | 6.985577 | -0.432107 | 0.671052 |
| H | 4.704573 | -0.890706 | 1.28490 |
| H | 3.780736 | -0.600293 | 2.54064 |
| H | 0.221021 | -1.665311 | 1.81569 |
| H | 1.615671 | -2.382461 | 1.82563 |
| H | -2.128961 | -1.521941 | -2.76218 |
| H | -1.975066 | -2.675735 | -1.71825 |
| H | -5.288415 | -1.045475 | -1.12595 |
| H | -5.046938 | -1.896104 | 0.162188 |
| H | -4.785068 | 1.795825 | 1.01930 |
| H | -4.398234 | 0.929764 | 2.26287 |
| H | -1.893518 | 2.442744 | 1.69880 |
| H | -0.477699 | 1.869865 | 1.33337 |

B3LYP optimized without symmetry constraints

E(B3LYP, small basis, gas)=-1197.31849119

**(COMPLEX B4)**

| | | | |
|---|---|---|---|
| U | 2.061935 | 0.071282 | 0.069805 |
| U | -2.482830 | 0.012871 | -0.004251 |
| F | -0.238487 | 0.130053 | 0.616278 |
| O | 2.578334 | -0.882651 | 1.470992 |
| O | 1.470560 | 1.072697 | -1.299729 |
| O | 1.871480 | 1.970750 | 1.612878 |
| O | 4.248374 | 1.136544 | 0.111899 |
| O | 6.075536 | -0.796879 | -0.304142 |
| O | 3.622167 | -1.174132 | -1.314809 |
| O | 0.939007 | -1.947191 | -0.794664 |
| O | -3.110110 | 1.429629 | 0.849980 |
| O | -1.946074 | -1.423236 | -0.934849 |

| | | | |
|---|---|---|---|
| O | -2.084991 | -1.109990 | 2.158327 |
| O | -4.528840 | -1.169954 | 0.689540 |
| O | -4.068130 | 0.589155 | -1.788766 |
| O | -1.306902 | 1.497547 | -1.566651 |
| H | 2.255152 | 1.946647 | 2.506919 |
| H | 1.405337 | 2.811481 | 1.469537 |
| H | 5.072497 | 0.580084 | 0.072478 |
| H | 4.448243 | 2.085184 | 0.080070 |
| H | 6.394140 | -1.334904 | 0.443015 |
| H | 6.814040 | -0.619630 | -0.914860 |
| H | 4.578822 | -1.248820 | -1.042101 |
| H | 3.486216 | -1.447932 | -2.235870 |
| H | -0.003849 | -2.002513 | -1.048368 |
| H | 1.350088 | -2.827139 | -0.781689 |
| H | -1.229422 | -1.081942 | 2.615080 |
| H | -2.753656 | -1.555517 | 2.703281 |
| H | -5.260992 | -0.751420 | 1.176630 |
| H | -4.787121 | -2.063411 | 0.401354 |
| H | -4.763984 | 1.265697 | -1.711743 |
| H | -4.156219 | 0.113908 | -2.633759 |
| H | -1.727624 | 2.196810 | -2.091916 |
| H | -0.336210 | 1.482554 | -1.705565 |

RI-MP2 optimized without symmetry constraints
E(RI-MP2, large basis, no ECP on O, gas phase)= -2036.0754040691

| | | | |
|---|---|---|---|
| U | 2.1178934 | 0.0980678 | 0.0372626 |
| U | -2.4340048 | -0.0353828 | 0.0217615 |
| F | -0.1706372 | 0.0245523 | 0.4222669 |
| O | 2.4986327 | -1.2880874 | 1.0864410 |
| O | 1.7664452 | 1.5453107 | -0.9595174 |
| O | 1.8689944 | 1.4643508 | 2.0663735 |
| O | 4.3592414 | 0.9104468 | 0.5826804 |
| O | 5.9985588 | -1.1321618 | -0.1803261 |
| O | 3.6951529 | -0.8379362 | -1.6042904 |
| O | 1.0301032 | -1.4176324 | -1.6205192 |
| O | -2.8427735 | 1.1808390 | 1.2534838 |
| O | -2.1221618 | -1.3397260 | -1.1641762 |
| O | -2.1092472 | -1.6066715 | 1.8861911 |
| O | -4.6468075 | -1.0569062 | 0.4137240 |
| O | -3.9965718 | 1.1156525 | -1.5386808 |
| O | -1.2960936 | 1.6499134 | -1.4199450 |
| H | 2.2084803 | 1.1974907 | 2.9365119 |
| H | 1.6305432 | 2.4013285 | 2.1496808 |
| H | 5.1161742 | 0.2834823 | 0.4972414 |
| H | 4.7200957 | 1.8084918 | 0.5264773 |
| H | 6.1530721 | -1.9009383 | 0.3942569 |
| H | 6.8695103 | -0.9721627 | -0.5823988 |
| H | 4.5720541 | -1.1213004 | -1.2430359 |
| H | 3.8744112 | -0.4483414 | -2.4750754 |
| H | 0.0981176 | -1.6709803 | -1.7081112 |
| H | 1.5494314 | -2.0928937 | -2.0841236 |
| H | -2.2072719 | -1.3793849 | 2.8252064 |
| H | -2.0003766 | -2.5706522 | 1.8555534 |
| H | -5.3029801 | -0.7848685 | 1.0767788 |
| H | -5.0227603 | -1.8387015 | -0.0235749 |
| H | -4.6474652 | 1.7800288 | -1.2553635 |
| H | -4.3467740 | 0.7481495 | -2.3675614 |
| H | -1.7576054 | 2.2777980 | -1.9959224 |
| H | -0.3626960 | 1.9161929 | -1.3993009 |

***Associative-Transition State geometry 2***
B3LYP optimized without symmetry constraints

E(B3LYP, small basis, gas)= -1197.29675704

**(COMPLEX TB4)**

| | | | |
|---|---|---|---|
| U | -2.440033 | -0.017211 | -0.024609 |
| U | 2.187806 | -0.020876 | 0.063557 |
| F | -0.134594 | -0.324547 | -0.065437 |
| O | -2.168953 | -2.458506 | 0.050508 |
| O | -1.214272 | 2.125574 | -0.107815 |
| O | -2.433535 | 0.009389 | 1.752904 |
| O | -2.567132 | -0.129959 | -1.792110 |
| O | -4.724642 | -0.930417 | 0.117027 |
| O | -3.979298 | 1.941158 | -0.119789 |
| O | 2.437507 | -1.767274 | 0.297820 |
| O | 1.610761 | 1.686567 | 0.102400 |
| O | 3.981205 | 0.770924 | 1.524534 |
| O | 3.426663 | 1.291809 | -1.734206 |
| O | 1.373636 | -0.198592 | 2.376952 |
| O | 1.694472 | -0.854290 | -2.218949 |
| O | 4.771951 | -0.873883 | -0.444821 |
| H | -5.187288 | -1.136639 | 0.947391 |
| H | -5.290330 | -1.148581 | -0.643470 |
| H | -4.410862 | 2.345429 | 0.653038 |
| H | -4.403675 | 2.251280 | -0.938836 |
| H | -2.057329 | -2.980779 | 0.862262 |
| H | -2.242232 | -3.045207 | -0.720709 |
| H | -1.644455 | 2.991152 | -0.178817 |
| H | -0.240211 | 2.203096 | -0.062906 |
| H | 4.834570 | 0.308112 | 1.483090 |
| H | 4.035806 | 0.978246 | -2.421701 |
| H | 3.997137 | 1.509917 | 2.153704 |
| H | 3.367944 | 2.261938 | -1.740511 |
| H | 1.554838 | -0.984507 | 2.919337 |
| H | 1.633123 | -1.804863 | -2.409081 |
| H | 0.866513 | 0.456320 | 2.883581 |
| H | 1.502535 | -0.330526 | -3.013748 |
| H | 4.854233 | -1.839391 | -0.354989 |
| H | 5.578972 | -0.510065 | -0.847510 |

***Dissociative-Intermediate geometry***

SCF optimized in $C_s$ symmetry

E(SCF, small basis, gas)= -1189.33684591

| | | | |
|---|---|---|---|
| U | 0.779838 | -2.745340 | 0.000000 |
| U | -0.882452 | 2.945664 | 0.000000 |
| F | -0.823560 | 0.633992 | 0.000000 |
| O | -0.199084 | -4.145246 | 0.000000 |
| O | 1.755148 | -1.323922 | 0.000000 |
| O | -0.703019 | -1.563406 | 1.499020 |
| O | -0.703019 | -1.563406 | -1.499020 |
| O | 2.220798 | -3.948636 | 1.520119 |
| O | 2.220798 | -3.948636 | -1.520119 |
| O | 2.349409 | -6.274478 | 0.000000 |
| O | -0.914802 | 2.981932 | 1.718631 |
| O | -0.914802 | 2.981932 | -1.718631 |
| O | -3.288027 | 2.322940 | 0.000000 |
| O | -2.158064 | 5.089733 | 0.000000 |
| O | 0.818058 | 4.792300 | 0.000000 |
| O | 1.449160 | 2.052628 | 0.000000 |
| H | -1.264031 | -1.871543 | 2.201537 |
| H | -1.264031 | -1.871543 | -2.201537 |
| H | -0.861341 | -0.641219 | 1.266011 |
| H | -0.861341 | -0.641219 | -1.266011 |
| H | 2.321873 | -4.887275 | 1.320872 |

| | | | |
|---|---|---|---|
| H | 2.321873 | -4.887275 | -1.320872 |
| H | 2.791851 | -3.667282 | 2.226447 |
| H | 2.791851 | -3.667282 | -2.226447 |
| H | 1.598029 | -6.858839 | 0.000000 |
| H | 3.155987 | -6.780217 | 0.000000 |
| H | -3.818770 | 2.222258 | 0.782518 |
| H | -3.818770 | 2.222258 | -0.782518 |
| H | -2.440332 | 5.552846 | 0.781821 |
| H | -2.440332 | 5.552846 | -0.781821 |
| H | 1.114660 | 5.245371 | 0.782816 |
| H | 1.114660 | 5.245371 | -0.782816 |
| H | 2.246755 | 2.565238 | 0.000000 |
| H | 1.622999 | 1.119297 | 0.000000 |

B3LYP optimized in $C_s$ symmetry
E(B3LYP, small basis, gas)= -1197.30938985
**(COMPLEX D2)**

| | | | |
|---|---|---|---|
| U | 0.721908 | -2.690530 | 0.000000 |
| U | -0.895121 | 2.871914 | 0.000000 |
| F | -0.978388 | 0.566769 | 0.000000 |
| O | -0.215778 | -4.189383 | 0.000000 |
| O | 1.638490 | -1.152595 | 0.000000 |
| O | -0.785803 | -1.583073 | 1.477811 |
| O | -0.785803 | -1.583073 | -1.477811 |
| O | 2.195371 | -3.843868 | 1.479095 |
| O | 2.195371 | -3.843868 | -1.479095 |
| O | 2.512692 | -6.080169 | 0.000000 |
| O | -0.945451 | 2.932944 | 1.775160 |
| O | -0.945451 | 2.932944 | -1.775160 |
| O | -3.308978 | 2.390029 | 0.000000 |
| O | -2.009432 | 5.076257 | 0.000000 |
| O | 0.931689 | 4.577424 | 0.000000 |
| O | 1.358525 | 1.847597 | 0.000000 |
| H | -1.382717 | -1.923066 | 2.164516 |
| H | -1.382717 | -1.923066 | -2.164516 |
| H | -0.973652 | -0.641435 | 1.223145 |
| H | -0.973652 | -0.641435 | -1.223145 |
| H | 2.360582 | -4.793673 | 1.222445 |
| H | 2.360582 | -4.793673 | -1.222445 |
| H | 2.759611 | -3.551188 | 2.213871 |
| H | 2.759611 | -3.551188 | -2.213871 |
| H | 1.800685 | -6.746426 | 0.000000 |
| H | 3.375931 | -6.533726 | 0.000000 |
| H | -3.859505 | 2.323796 | 0.797976 |
| H | -3.859505 | 2.323796 | -0.797976 |
| H | -2.271349 | 5.567111 | 0.797449 |
| H | -2.271349 | 5.567111 | -0.797449 |
| H | 1.241964 | 5.039740 | 0.797712 |
| H | 1.241964 | 5.039740 | -0.797712 |
| H | 2.180218 | 2.361075 | 0.000000 |
| H | 1.529108 | 0.887949 | 0.000000 |

RI-MP2 optimized in $C_s$ symmetry
E(RI-MP2, large basis, no ECP on O, gas phase)= -2036.0550200219

| | | | |
|---|---|---|---|
| U | -0.0513875 | -2.8575554 | 0.0000000 |
| U | 0.0239549 | 3.0306406 | 0.0000000 |
| F | -0.5997423 | 0.8391355 | 0.0000000 |
| O | -1.5018064 | -3.8813357 | 0.0000000 |
| O | 1.3803526 | -1.7880865 | 0.0000000 |
| O | -1.0319388 | -1.2508338 | 1.4981149 |
| O | -1.0319388 | -1.2508338 | -1.4981149 |
| O | 0.8488408 | -4.4692714 | 1.5377857 |

| | | | |
|---|---|---|---|
| O | 0.8488408 | -4.4692714 | -1.5377857 |
| O | 0.2672928 | -6.6544897 | 0.0000000 |
| O | -0.0155007 | 3.1167967 | 1.7801848 |
| O | -0.0155007 | 3.1167967 | -1.7801848 |
| O | -2.4471040 | 3.1699894 | 0.0000000 |
| O | -0.5302548 | 5.4525090 | 0.0000000 |
| O | 2.2100851 | 4.2513689 | 0.0000000 |
| O | 2.0172631 | 1.5240814 | 0.0000000 |
| H | -1.8264954 | -1.2998627 | 2.0530535 |
| H | -1.8264954 | -1.2998627 | -2.0530538 |
| H | -0.9294210 | -0.3211068 | 1.1688515 |
| H | -0.9294210 | -0.3211068 | -1.1688515 |
| H | 0.6337891 | -5.4017540 | 1.2877399 |
| H | 0.6337891 | -5.4017540 | -1.2877399 |
| H | 1.6015034 | -4.4854516 | 2.1511650 |
| H | 1.6015034 | -4.4854516 | -2.1511650 |
| H | -0.6218742 | -7.0486343 | 0.0000000 |
| H | 0.8531316 | -7.4310629 | 0.0000000 |
| H | -3.0046482 | 3.3480076 | 0.7738590 |
| H | -3.0046482 | 3.3480076 | -0.7738590 |
| H | -0.6772599 | 6.0191456 | 0.7743526 |
| H | -0.6772599 | 6.0191456 | -0.7743526 |
| H | 2.5748486 | 4.7127264 | 0.7729662 |
| H | 2.5748486 | 4.7127264 | -0.7729662 |
| H | 2.9410256 | 1.8131147 | 0.0000000 |
| H | 2.0141120 | 0.5563891 | 0.0000000 |

***Dissociative-Transition State geometry***
B3LYP optimized without symmetry constraints
E(B3LYP, small basis, gas)= -1197.30369598
**(COMPLEX TD2)**

| | | | |
|---|---|---|---|
| U | 2.974616 | 0.032746 | -0.009356 |
| U | -2.873222 | -0.081827 | 0.041372 |
| F | 0.803912 | -0.738375 | -0.078155 |
| O | 3.248219 | -2.395954 | -0.278525 |
| O | 1.308557 | 1.850273 | 0.249257 |
| O | 3.017524 | 0.209744 | -1.777142 |
| O | 3.079657 | -0.203168 | 1.748570 |
| O | 5.414305 | -0.344100 | -0.092611 |
| O | 4.034403 | 2.284592 | 0.220578 |
| O | -3.991144 | -1.444217 | -0.093794 |
| O | -1.674639 | 1.228635 | 0.272697 |
| O | -3.730709 | 1.016733 | -1.888150 |
| O | -3.852494 | 0.475367 | 2.185992 |
| O | -1.333635 | -0.972892 | -1.556645 |
| O | -1.322072 | -1.422729 | 1.269889 |
| O | -5.837122 | 0.792518 | -0.488798 |
| H | 5.948753 | -0.346383 | -0.904899 |
| H | 5.973818 | -0.540054 | 0.678113 |
| H | 4.357096 | 2.809968 | -0.531930 |
| H | 4.404754 | 2.627675 | 1.052184 |
| H | 3.331526 | -2.853946 | -1.131564 |
| H | 3.370294 | -3.021515 | 0.455048 |
| H | 0.343682 | 1.715995 | 0.270117 |
| H | 1.546506 | 2.783903 | 0.352045 |
| H | -4.718552 | 1.069319 | -1.802134 |
| H | -4.638829 | 0.039602 | 2.560134 |
| H | -3.362719 | 1.482856 | -2.654748 |
| H | -3.516344 | 1.147318 | 2.805079 |
| H | -1.491274 | -1.534376 | -2.332687 |
| H | -1.470877 | -2.209152 | 1.818970 |

| | | | |
|---|---|---|---|
| H | -0.378510 | -0.928654 | -1.288867 |
| H | -0.367582 | -1.281122 | 1.036823 |
| H | -6.432726 | 0.027279 | -0.579804 |
| H | -6.349298 | 1.573681 | -0.214479 |

## Total water molecules 10

***Precursor geometry***

DFT-optimized without symmetry constraints

E(B3LYP,small basis, gas phase)= -1214.59497966

(**COMPLEX P1**)

| | | | |
|---|---|---|---|
| U | -3.024923 | -0.114732 | 0.015544 |
| U | 3.532389 | 0.049598 | -0.007111 |
| F | -0.715964 | -0.125105 | 0.002904 |
| O | -2.456767 | -0.631732 | -2.345223 |
| O | -2.422241 | 0.146017 | 2.407224 |
| O | -3.003641 | -1.870579 | 0.295386 |
| O | -2.961400 | 1.640749 | -0.261898 |
| O | -5.068354 | -0.202379 | -1.354857 |
| O | -5.051246 | 0.203008 | 1.374895 |
| O | 3.655984 | -0.197463 | -1.759540 |
| O | 3.622704 | 0.303047 | 1.746440 |
| O | 4.230643 | -2.305092 | 0.327224 |
| O | 4.032049 | 2.450138 | -0.362109 |
| O | 1.553512 | -1.386964 | 0.175385 |
| O | 1.444284 | 1.315959 | -0.195670 |
| O | 5.987967 | 0.158087 | 0.011887 |
| H | -5.911773 | 0.252166 | -1.094943 |
| H | -5.180488 | -0.748398 | -2.146810 |
| H | -5.157735 | -0.111328 | 2.284676 |
| H | -5.898082 | 0.568253 | 1.007570 |
| H | -2.184553 | -1.509737 | -2.658373 |
| H | -2.397437 | 0.024300 | -3.059135 |
| H | -2.120099 | -0.578417 | 2.978900 |
| H | -2.389876 | 0.995146 | 2.877716 |
| H | 4.494609 | -2.902890 | -0.393569 |
| H | 4.253729 | 2.836102 | -1.227238 |
| H | 4.482517 | -2.682961 | 1.187657 |
| H | 4.241318 | 3.078156 | 0.350834 |
| H | 1.619832 | -2.344564 | 0.301882 |
| H | 1.430031 | 2.273104 | -0.340662 |
| H | 0.609596 | -1.077383 | 0.130334 |
| H | 0.529295 | 0.930675 | -0.141221 |
| H | 6.556704 | 0.067754 | -0.771845 |
| H | 6.529950 | 0.298081 | 0.807209 |
| H | -7.979669 | 0.566673 | -0.054858 |
| O | -7.125590 | 1.027819 | -0.129828 |
| H | -7.274272 | 1.978680 | -0.274616 |

***Asociative Intermediate geometry***

DFT-optimized without symmetry constraints

E(B3LYP,small basis, gas phase)= -1214.57650094

(**COMPLEX B1**)

| | | | |
|---|---|---|---|
| U | 2.221657 | -0.141336 | -0.065031 |
| U | -2.391964 | -0.021864 | 0.018451 |
| F | -0.094898 | -0.381312 | 0.184706 |
| O | 2.086548 | -2.449169 | 0.783475 |
| O | 1.064657 | 1.968770 | -0.616971 |
| O | 2.024182 | -0.796858 | -1.706516 |
| O | 2.434569 | 0.432803 | 1.603855 |
| O | 4.525058 | -0.963762 | 0.104241 |

| | | | |
|---|---|---|---|
| O | 3.799187 | 1.568114 | -0.844492 |
| O | -2.649482 | -1.723345 | 0.478922 |
| O | -1.765472 | 1.568175 | -0.566890 |
| O | -3.931281 | 0.625152 | -1.875853 |
| O | -3.599377 | 1.852191 | 1.298765 |
| O | -1.734787 | -1.208922 | -2.036016 |
| O | -1.823573 | 0.033737 | 2.422095 |
| O | -4.879306 | -0.475690 | 0.516405 |
| H | 4.879874 | -1.815740 | -0.192023 |
| H | 5.238557 | -0.340793 | 0.396145 |
| H | 4.646077 | 1.693208 | -0.336157 |
| H | 3.883955 | 1.877891 | -1.760464 |
| H | 1.844184 | -3.233990 | 0.265286 |
| H | 2.308597 | -2.697426 | 1.696566 |
| H | 1.513495 | 2.827576 | -0.631263 |
| H | 0.095229 | 2.054151 | -0.711331 |
| H | -4.636469 | 0.086085 | -2.270409 |
| H | -4.253427 | 1.759719 | 2.010558 |
| H | -3.852468 | 1.477350 | -2.335273 |
| H | -3.466803 | 2.786094 | 1.067034 |
| H | -1.674809 | -2.177986 | -2.053116 |
| H | -1.693730 | -0.784447 | 2.928688 |
| H | -1.499197 | -0.834177 | -2.899930 |
| H | -1.655096 | 0.814942 | 2.972550 |
| H | -5.122972 | -1.365709 | 0.822887 |
| H | -5.666760 | 0.082082 | 0.408926 |
| H | 6.077387 | 1.569714 | 1.540381 |
| O | 6.030968 | 1.235676 | 0.626900 |
| H | 6.901517 | 1.332656 | 0.200663 |

***Dissociative Intermediate geometry***

DFT-optimized without symmetry constraints

E(B3LYP,small basis, gas phase)= -1214.58714602

(**COMPLEX D1**)

| | | | |
|---|---|---|---|
| U | 2.978442 | 0.065030 | 0.010547 |
| U | -2.774980 | 0.089411 | -0.023292 |
| F | -0.567081 | 0.796320 | -0.004276 |
| O | 4.163058 | 1.378187 | 0.068582 |
| O | 1.760405 | -1.243096 | -0.049617 |
| O | 1.519447 | 1.262940 | -1.444558 |
| O | 1.486206 | 1.168019 | 1.502300 |
| O | 4.514911 | -0.984404 | -1.485505 |
| O | 4.478792 | -1.080897 | 1.471586 |
| O | 6.735417 | -0.714792 | 0.030913 |
| O | -2.755149 | 0.233424 | -1.793525 |
| O | -2.706403 | 0.113023 | 1.752475 |
| O | -3.037478 | 2.541963 | 0.029811 |
| O | -5.176332 | 0.638349 | 0.056775 |
| O | -4.180129 | -1.945718 | -0.090580 |
| O | -1.203506 | -1.854721 | -0.154283 |
| H | 1.662773 | 1.867403 | -2.190967 |
| H | 1.612842 | 1.726638 | 2.286349 |
| H | 0.559498 | 1.157020 | -1.200615 |
| H | 0.530536 | 1.081920 | 1.225658 |
| H | 5.469385 | -0.887856 | -1.214253 |
| H | 5.439552 | -0.967581 | 1.230898 |
| H | 4.398825 | -1.583676 | -2.241110 |
| H | 4.343987 | -1.728090 | 2.183259 |
| H | 7.173375 | 0.155666 | 0.064233 |
| H | 7.413582 | -1.415107 | 0.016298 |
| H | -3.053077 | 3.111993 | -0.757091 |
| H | -3.025885 | 3.080721 | 0.837944 |

| | | | |
|---|---|---|---|
| H | -5.932232 | 0.002833 | 0.092252 |
| H | -5.489879 | 1.556515 | 0.062387 |
| H | -5.163770 | -1.911357 | 0.026352 |
| H | -3.914202 | -2.805914 | -0.453534 |
| H | -1.410081 | -2.794498 | -0.036404 |
| H | -0.239184 | -1.713180 | -0.129787 |
| H | -7.192312 | -1.687617 | 1.068397 |
| O | -6.774232 | -1.500293 | 0.210920 |
| H | -7.398573 | -1.717091 | -0.501661 |

***Intermediate following a dissociation of water from A-intermediate***
DFT-optimized without symmetry constraints
E(B3LYP,small basis, gas phase)= -1214.60026587
(**COMPLEX B3**)

| | | | |
|---|---|---|---|
| U | 2.262118 | 0.095739 | 0.016026 |
| U | -2.263458 | -0.041840 | 0.098301 |
| F | 0.004300 | 0.278536 | 0.597755 |
| O | 2.109451 | 2.253849 | 1.180379 |
| O | 1.165701 | -2.063670 | -0.399041 |
| O | 2.892902 | -0.563694 | 1.536125 |
| O | 1.623836 | 0.790523 | -1.514581 |
| O | 4.423486 | 1.201598 | -0.212777 |
| O | 3.817087 | -1.371810 | -1.142437 |
| O | -2.867470 | 1.524475 | 0.667621 |
| O | -1.623092 | -1.636088 | -0.431670 |
| O | -4.428906 | -0.965518 | 0.732622 |
| O | -3.814977 | 0.095650 | -1.774255 |
| O | -2.085049 | -0.642144 | 2.471586 |
| O | -1.169792 | 1.131023 | -1.765797 |
| O | -6.274566 | 0.352242 | -0.729564 |
| H | 5.249471 | 0.668062 | -0.079552 |
| H | 4.610981 | 2.087802 | -0.559633 |
| H | 3.707919 | -1.767875 | -2.021355 |
| H | 4.766037 | -1.391885 | -0.836501 |
| H | 1.506692 | 2.993077 | 1.001170 |
| H | 2.674852 | 2.454044 | 1.945646 |
| H | 1.619826 | -2.915953 | -0.303544 |
| H | 0.203527 | -2.180290 | -0.546768 |
| H | -5.261183 | -0.559001 | 0.372503 |
| H | -4.775449 | 0.299297 | -1.603265 |
| H | -4.606397 | -1.762863 | 1.255044 |
| H | -3.674153 | -0.257945 | -2.666876 |
| H | -2.488970 | -0.088648 | 3.162182 |
| H | -1.613558 | 1.792292 | -2.320494 |
| H | -1.571477 | -1.362412 | 2.872895 |
| H | -0.206703 | 1.093957 | -1.947655 |
| H | -6.588515 | 1.222254 | -0.424067 |
| H | -7.016470 | -0.141776 | -1.123056 |
| H | 6.499710 | -1.197391 | 0.727862 |
| O | 6.236122 | -0.815581 | -0.128672 |
| H | 7.010584 | -0.777137 | -0.718717 |

***Intermediate having 6-coordinated $U_A$ and $U_B$***
DFT-optimized without symmetry constraints
E(B3LYP,small basis, gas phase)= -1214.55620071
(**COMPLEX B5**)

| | | | |
|---|---|---|---|
| U | -2.298133 | -0.030400 | 0.092539 |
| U | 2.286537 | -0.018110 | 0.012969 |
| F | 0.000796 | 0.007363 | 0.500180 |
| O | -1.109768 | 1.592631 | -1.313946 |

| | | | |
|---|---|---|---|
| O | -1.864597 | -1.653753 | 1.880240 |
| O | -1.775916 | -1.360635 | -1.010374 |
| O | -2.535344 | 1.078438 | 1.465608 |
| O | -3.709475 | 2.109754 | -0.626247 |
| O | -4.485569 | -0.911391 | 0.830626 |
| O | 1.718682 | 1.197921 | -1.191793 |
| O | 2.503889 | -1.256134 | 1.270040 |
| O | 3.752402 | -1.746297 | -1.126417 |
| O | 4.373969 | 0.559178 | 1.431847 |
| O | 1.033367 | -1.653319 | -1.344125 |
| O | 1.891054 | 1.788199 | 1.638325 |
| O | 4.280455 | 0.983213 | -1.315220 |
| H | -3.885908 | 2.707741 | 0.120497 |
| H | -4.245203 | 2.367160 | -1.394379 |
| H | -4.874778 | -0.738075 | 1.703920 |
| H | -5.045999 | -1.516130 | 0.318142 |
| H | -0.153575 | 1.572491 | -1.522444 |
| H | -1.552564 | 2.383910 | -1.655219 |
| H | -1.770040 | -1.404298 | 2.814143 |
| H | -1.719183 | -2.606581 | 1.763167 |
| H | 4.278678 | -1.619229 | -1.932619 |
| H | 4.957955 | 1.335080 | 1.416353 |
| H | 3.998124 | -2.573111 | -0.677740 |
| H | 4.675695 | -0.088307 | 2.091420 |
| H | 0.057163 | -1.710856 | -1.382460 |
| H | 1.278854 | 2.531599 | 1.523944 |
| H | 1.463131 | -2.348760 | -1.863079 |
| H | 2.299500 | 1.805917 | 2.518626 |
| H | 4.065658 | 1.652365 | -1.986669 |
| H | 5.241774 | 0.875042 | -1.229516 |
| H | -4.876938 | -0.015580 | -2.066032 |
| O | -3.999553 | -0.379369 | -1.864850 |
| H | -3.721423 | -1.001202 | -2.558176 |