**$H_2O$**

| | | | | |
|---|---|---|---|---|
| 1 | O | 1.204947 | -0.15585 | 0 |
| 2 | H | 2.169864 | -0.11187 | 0 |
| 3 | H | 0.924309 | 0.768401 | 0 |

**$(H_2O)_3$**

| | | | | |
|---|---|---|---|---|
| 1 | O | 0.638605 | 2.529956 | -1.82825 |
| 2 | H | 0.715452 | 3.432654 | -1.46878 |
| 3 | H | 0.698549 | 2.631403 | -2.79574 |
| 4 | O | 0.8627 | 5.17221 | -0.71243 |
| 5 | O | 0.80897 | 2.771482 | -4.69072 |
| 6 | H | 1.600422 | 5.293277 | -0.09983 |
| 7 | H | 0.08647 | 5.475916 | -0.22316 |
| 8 | H | 1.561402 | 2.315555 | -5.09087 |
| 9 | H | 0.03944 | 2.445391 | -5.17617 |

**$(H_2O)_6$**

| | | | | |
|---|---|---|---|---|
| 1 | O | -3.02454 | 0.252353 | -1.02805 |
| 2 | H | -3.45661 | -0.56219 | -0.70814 |
| 3 | H | -3.28854 | 0.949727 | -0.39544 |
| 4 | H | -6.35459 | -1.79826 | 2.376918 |
| 5 | O | -6.5691 | -1.92287 | 1.441726 |
| 6 | H | -7.12346 | -2.71557 | 1.417683 |
| 7 | H | -8.74851 | 0.343059 | 0.516394 |
| 8 | O | -7.80669 | 0.358255 | 0.304385 |
| 9 | H | -7.43224 | -0.44163 | 0.725616 |
| 10 | H | -6.82415 | 3.106275 | 1.594689 |
| 11 | O | -6.46688 | 2.701675 | 0.794524 |
| 12 | H | -6.97663 | 1.867251 | 0.67118 |
| 13 | H | -3.42873 | 2.233742 | 1.633251 |
| 14 | O | -3.74159 | 2.359138 | 0.728863 |
| 15 | H | -4.71701 | 2.478491 | 0.806347 |
| 16 | H | -3.65208 | -2.82253 | 0.207316 |
| 17 | O | -4.25474 | -2.19868 | -0.21658 |
| 18 | H | -5.02183 | -2.13781 | 0.38539 |

**$H_3O^+$**

| | | | | |
|---|---|---|---|---|
| 1 | O | -2.2661 | 2.037335 | 0.162538 |
| 2 | H | -1.34315 | 1.952309 | 0.480091 |
| 3 | H | -2.65504 | 2.878646 | 0.480183 |
| 4 | H | -2.80237 | 1.279859 | 0.477189 |

**$Acet^-$**

| | | | | |
|---|---|---|---|---|
| 1 | C | -1.58864 | 0.448176 | -0.05945 |
| 2 | C | -0.23604 | -0.199 | 0.282348 |
| 3 | H | 0.391794 | 0.467268 | 0.88669 |
| 4 | H | -0.38876 | -1.14752 | 0.815883 |
| 5 | O | -1.72757 | 1.683795 | 0.183182 |
| 6 | O | -2.46552 | -0.30711 | -0.57684 |
| 7 | H | 0.297728 | -0.43291 | -0.65137 |

**$[UO_2(H_2O)_5]^{2+}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.92178 | -0.03979 | 0.00207 |
| 2 | O | -0.92941 | 0.029833 | -1.75768 |
| 3 | O | -0.89563 | -0.06787 | 1.762814 |
| 4 | O | 1.104584 | 1.324425 | 0.171019 |
| 5 | O | -3.38427 | -0.2742 | 0.029927 |
| 6 | O | -1.69334 | -2.42054 | -0.03129 |
| 7 | H | 1.549884 | 1.575301 | 0.992387 |
| 8 | H | 1.617117 | 1.694371 | -0.56174 |
| 9 | H | -3.95603 | -0.05512 | -0.72042 |
| 10 | H | -3.92123 | -0.17929 | 0.830318 |
| 11 | H | -1.12047 | -3.15998 | -0.27665 |
| 12 | H | -2.60694 | -2.67142 | -0.22487 |
| 13 | H | 1.470528 | -1.92477 | 0.671753 |
| 14 | O | 0.947865 | -1.6544 | -0.09724 |
| 15 | H | 1.502205 | -1.79349 | -0.87894 |
| 16 | O | -1.77654 | 2.258254 | -0.04994 |
| 17 | H | -1.96773 | 2.77318 | -0.84638 |
| 18 | H | -1.94982 | 2.827949 | 0.712913 |

**$[UO_2(H_2O)_3(Ac)]^+$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -1.04173 | -0.26989 | -0.09961 |
| 2 | O | -1.16151 | -0.09765 | -1.86066 |
| 3 | O | -1.03286 | -0.42683 | 1.666407 |
| 4 | O | -3.51636 | -0.03322 | 0.066907 |
| 5 | O | -1.77854 | -2.62331 | -0.30505 |
| 6 | H | -4.13401 | 0.095384 | -0.66601 |
| 7 | H | -4.03824 | -0.05329 | 0.880659 |
| 8 | H | -1.85389 | -3.11601 | -1.1338 |
| 9 | H | -1.81058 | -3.2687 | 0.414336 |
| 10 | O | -1.3201 | 2.177082 | 0.131477 |
| 11 | H | -1.29274 | 2.816279 | -0.59363 |
| 12 | H | -1.24407 | 2.677275 | 0.955565 |
| 13 | C | 1.757443 | -0.52147 | -0.18405 |
| 14 | C | 3.246971 | -0.66682 | -0.16599 |
| 15 | H | 3.728686 | 0.27293 | -0.45354 |

| | | | | |
|---|---|---|---|---|
| 16 | H | 3.553879 | -0.92096 | 0.859356 |
| 17 | O | 1.198022 | 0.622889 | -0.06939 |
| 18 | O | 0.994438 | -1.5436 | -0.28625 |
| 19 | H | 3.555998 | -1.48499 | -0.82573 |

**$[UO_2(H_2O)(Ac)_2]^0$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.51086 | 0.558744 | -0.16614 |
| 2 | O | -0.69498 | 0.286795 | -1.9199 |
| 3 | O | -0.36687 | 0.759478 | 1.600748 |
| 4 | O | -1.69179 | -1.62423 | 0.2708 |
| 5 | H | -2.62516 | -1.67713 | 0.022767 |
| 6 | H | -1.25782 | -2.43265 | -0.03515 |
| 7 | C | 2.02802 | -0.73945 | -0.25781 |
| 8 | C | 3.366769 | -1.41618 | -0.3047 |
| 9 | H | 3.706951 | -1.58544 | 0.727382 |
| 10 | H | 3.280804 | -2.39144 | -0.79724 |
| 11 | O | 1.928278 | 0.52853 | -0.37828 |
| 12 | O | 0.961002 | -1.41642 | -0.07667 |
| 13 | H | 4.099908 | -0.78504 | -0.81702 |
| 14 | C | -2.97934 | 1.989339 | -0.13036 |
| 15 | C | -4.2689 | 2.756983 | -0.12251 |
| 16 | H | -4.11148 | 3.759145 | 0.291345 |
| 17 | H | -4.61345 | 2.866812 | -1.16123 |
| 18 | O | -1.86701 | 2.586288 | -0.33012 |
| 19 | O | -2.9651 | 0.725191 | 0.042282 |
| 20 | H | -5.0347 | 2.217298 | 0.444145 |

**$[UO_2(Ac)_3]^-$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -1.16733 | -0.39282 | -0.45282 |
| 2 | O | -0.95921 | -0.07549 | -2.20663 |
| 3 | O | -1.37567 | -0.70971 | 1.301026 |
| 4 | C | 1.707718 | -0.42545 | -0.13394 |
| 5 | C | 3.209517 | -0.43423 | -0.02493 |
| 6 | H | 3.554468 | 0.375657 | 0.626868 |
| 7 | H | 3.563367 | -1.40395 | 0.342004 |
| 8 | O | 1.0533 | 0.659179 | 0.001272 |
| 9 | O | 1.070569 | -1.49845 | -0.39089 |
| 10 | H | 3.631577 | -0.27284 | -1.02793 |
| 11 | C | -2.63009 | 2.08656 | -0.16524 |
| 12 | C | -3.3961 | 3.366439 | 0.041104 |
| 13 | H | -2.78494 | 4.230723 | -0.24138 |
| 14 | H | -4.33259 | 3.352376 | -0.52674 |
| 15 | O | -1.36324 | 2.061246 | -0.03137 |
| 16 | O | -3.23879 | 1.004078 | -0.44917 |
| 17 | H | -3.64172 | 3.455893 | 1.109674 |

| | | | | |
|---|---|---|---|---|
| 18 | C | -2.57816 | -2.83967 | -1.07588 |
| 19 | C | -3.30879 | -4.10141 | -1.4521 |
| 20 | H | -2.75893 | -4.98407 | -1.10843 |
| 21 | H | -4.32471 | -4.0942 | -1.04186 |
| 22 | O | -1.31367 | -2.84243 | -0.92118 |
| 23 | O | -3.21127 | -1.74312 | -0.93331 |
| 24 | H | -3.3837 | -4.14604 | -2.5487 |

**$[UO_2[H_2O\text{---}(H_2O)_2]_5]^{2+}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | 0.182483 | 0.002512 | 0.045154 |
| 2 | O | 0.245094 | 0.03085 | 1.819815 |
| 3 | O | 0.185342 | -0.02684 | -1.73092 |
| 4 | O | 2.139196 | 1.455525 | -0.00491 |
| 5 | H | 2.779372 | 1.451511 | 0.759458 |
| 6 | H | 2.664519 | 1.561338 | -0.82799 |
| 7 | H | 2.753124 | -1.45617 | -0.75452 |
| 8 | O | 2.13167 | -1.45937 | 0.025253 |
| 9 | H | 2.675592 | -1.57191 | 0.835314 |
| 10 | O | -2.32575 | 0.011962 | 0.102273 |
| 11 | H | -2.90999 | -0.77849 | 0.113948 |
| 12 | H | -2.90462 | 0.805779 | 0.069537 |
| 13 | H | -1.09674 | 2.695094 | 0.819615 |
| 14 | O | -0.66167 | 2.277511 | 0.026837 |
| 15 | H | -1.06447 | 2.700231 | -0.76285 |
| 16 | H | -1.07769 | -2.72427 | -0.62592 |
| 17 | O | -0.67215 | -2.26621 | 0.14246 |
| 18 | H | -1.11108 | -2.64143 | 0.954089 |
| 19 | H | -2.14427 | -2.87756 | 2.986593 |
| 20 | O | -2.15579 | -3.28346 | 2.109912 |
| 21 | H | -2.988 | -2.99113 | 1.688804 |
| 22 | H | -2.23149 | -3.19445 | -2.69025 |
| 23 | O | -2.24372 | -3.50841 | -1.77534 |
| 24 | H | -2.18389 | -4.47198 | -1.83677 |
| 25 | H | 3.80911 | -0.35027 | -2.3008 |
| 26 | O | 3.807888 | -1.29081 | -2.03152 |
| 27 | H | 3.611652 | -1.79575 | -2.83111 |
| 28 | H | 3.259451 | -1.87794 | 3.123663 |
| 29 | O | 3.688115 | -1.52727 | 2.33021 |
| 30 | H | 4.522071 | -2.01272 | 2.259064 |
| 31 | O | 3.865111 | 1.27757 | 2.011057 |
| 32 | H | 3.864134 | 0.337219 | 2.280963 |
| 33 | H | 3.692479 | 1.784519 | 2.81482 |
| 34 | O | 3.647369 | 1.514051 | -2.34207 |
| 35 | H | 3.209194 | 1.872656 | -3.12671 |
| 36 | H | 4.48702 | 1.991162 | -2.28212 |
| 37 | H | -2.1295 | 3.031257 | 2.838166 |

| | | | | |
|---|---|---|---|---|
| 38 | O | -2.13793 | 3.396153 | 1.943616 |
| 39 | H | -2.97169 | 3.089917 | 1.535786 |
| 40 | H | -2.2124 | 3.100493 | -2.85105 |
| 41 | O | -2.2234 | 3.444457 | -1.94692 |
| 42 | H | -2.15723 | 4.405154 | -2.03967 |
| 43 | H | -3.57028 | 2.789034 | -0.78104 |
| 44 | O | -3.87406 | 2.310803 | 0.016269 |
| 45 | H | -4.8346 | 2.239226 | -0.05476 |
| 46 | H | -3.58664 | -2.79536 | -0.6384 |
| 47 | O | -3.88691 | -2.27917 | 0.13631 |
| 48 | H | -4.84716 | -2.20581 | 0.063101 |

**$[UO_2(Ac)[H_2O\text{---}(H_2O)_2]_3]^+$**

| | | | | |
|---|---|---|---|---|
| 1 | U | 0.012849 | -0.03883 | 0.281745 |
| 2 | O | -0.11521 | -0.07194 | 2.056787 |
| 3 | O | 0.115196 | -0.00804 | -1.49648 |
| 4 | O | -2.49166 | -0.01716 | 0.153742 |
| 5 | H | -3.06939 | -0.8091 | 0.068326 |
| 6 | H | -3.05508 | 0.787394 | 0.095882 |
| 7 | H | -1.10551 | 2.697746 | 1.083319 |
| 8 | O | -0.61093 | 2.298351 | 0.315321 |
| 9 | H | -0.9376 | 2.762823 | -0.4872 |
| 10 | H | -0.9752 | -2.7953 | -0.58724 |
| 11 | O | -0.64357 | -2.36665 | 0.232834 |
| 12 | H | -1.14424 | -2.78904 | 0.984551 |
| 13 | H | -2.36825 | -3.13613 | 2.889264 |
| 14 | O | -2.30134 | -3.48453 | 1.990551 |
| 15 | H | -3.09361 | -3.16258 | 1.516786 |
| 16 | H | -1.96637 | -3.06609 | -2.75218 |
| 17 | O | -2.05951 | -3.46617 | -1.87625 |
| 18 | H | -2.00383 | -4.42046 | -2.02554 |
| 19 | H | -2.32668 | 2.973483 | 3.001201 |
| 20 | O | -2.25437 | 3.364757 | 2.120707 |
| 21 | H | -3.05017 | 3.076099 | 1.631614 |
| 22 | H | -1.92318 | 3.182764 | -2.63934 |
| 23 | O | -2.00856 | 3.519358 | -1.7363 |
| 24 | H | -1.93743 | 4.4809 | -1.81614 |
| 25 | H | -3.46045 | 2.85678 | -0.71572 |
| 26 | O | -3.86646 | 2.370705 | 0.030265 |
| 27 | H | -4.82092 | 2.390445 | -0.11668 |
| 28 | H | -3.49897 | -2.83746 | -0.81944 |
| 29 | O | -3.90039 | -2.37844 | -0.05398 |
| 30 | H | -4.85469 | -2.38017 | -0.20323 |
| 31 | O | 2.190709 | 1.041438 | 0.434287 |
| 32 | O | 2.177339 | -1.15041 | 0.396983 |
| 33 | C | 2.840653 | -0.05894 | 0.444138 |

| | | | | |
|---|---|---|---|---|
| 34 | C | 4.340034 | -0.069 | 0.478133 |
| 35 | H | 4.705806 | -0.9763 | 0.970335 |
| 36 | H | 4.707561 | -0.06708 | -0.5587 |
| 37 | H | 4.71831 | 0.828011 | 0.979395 |

**$[UO_2(Ac)_2[H_2O\text{---}(H_2O)_2]]^0$**

| | | | | |
|---|---|---|---|---|
| 1 | U | 0.544352 | 0.501557 | -0.62082 |
| 2 | O | 0.387183 | 1.427145 | 0.900203 |
| 3 | O | 0.665408 | -0.39599 | -2.16108 |
| 4 | O | 0.84799 | 2.569623 | -1.85096 |
| 5 | H | 0.814168 | 3.48082 | -1.46784 |
| 6 | H | 0.871612 | 2.638241 | -2.83717 |
| 7 | O | 0.770694 | 5.063998 | -0.83601 |
| 8 | O | 0.955211 | 2.746971 | -4.54283 |
| 9 | H | 1.486554 | 5.287512 | -0.22575 |
| 10 | H | -0.04147 | 5.29976 | -0.36738 |
| 11 | H | 1.162319 | 1.916798 | -4.99349 |
| 12 | H | 0.144928 | 3.064122 | -4.96453 |
| 13 | O | -1.73727 | 1.213757 | -1.24754 |
| 14 | O | -1.55153 | -0.65253 | -0.11381 |
| 15 | C | -2.29369 | 0.205322 | -0.69967 |
| 16 | C | -3.78232 | 0.014431 | -0.76695 |
| 17 | H | -4.01438 | -0.58341 | -1.66065 |
| 18 | H | -4.13891 | -0.53231 | 0.112635 |
| 19 | H | -4.29024 | 0.980419 | -0.85712 |
| 20 | O | 2.741405 | -0.33701 | 0.069699 |
| 21 | O | 1.021747 | -1.56829 | 0.648674 |
| 22 | C | 2.280559 | -1.37759 | 0.654496 |
| 23 | C | 3.209052 | -2.33051 | 1.351993 |
| 24 | H | 2.72946 | -3.30449 | 1.492262 |
| 25 | H | 4.141727 | -2.43433 | 0.785858 |
| 26 | H | 3.457236 | -1.91331 | 2.338907 |

**Glycolate$^-$**

| | | | | |
|---|---|---|---|---|
| 1 | C | -1.40883 | -0.56569 | 1.873317 |
| 2 | O | -0.15431 | -0.67984 | 1.724742 |
| 3 | O | -2.0424 | 0.443285 | 2.276899 |
| 4 | C | -2.22718 | -1.82147 | 1.510513 |
| 5 | O | -1.36858 | -2.87515 | 1.075823 |
| 6 | H | -0.48596 | -2.45279 | 1.144683 |
| 7 | H | -2.80361 | -2.14099 | 2.393626 |
| 8 | H | -2.94497 | -1.56362 | 0.715089 |

**$[UO_2(H_2O)_3(glycolate)]^+$**

| Tag | Symbol | X | Y | Z |
|---|---|---|---|---|
| 1 | U | -0.93431 | 0.086579 | 0.233328 |
| 2 | O | -0.55342 | -0.36944 | -1.43678 |
| 3 | O | -1.33777 | 0.641929 | 1.867056 |
| 4 | O | 0.947204 | 1.6864 | 0.180139 |
| 5 | O | -3.41346 | -0.0907 | -0.26717 |
| 6 | O | -1.92534 | -2.13756 | 0.68837 |
| 7 | H | 1.259665 | 2.232982 | 0.914111 |
| 8 | H | 1.55612 | 1.821214 | -0.55877 |
| 9 | H | -3.89269 | 0.715027 | -0.50655 |
| 10 | H | -3.99315 | -0.60679 | 0.310371 |
| 11 | H | -2.22808 | -2.68642 | -0.04828 |
| 12 | H | -1.25394 | -2.68344 | 1.205904 |
| 13 | O | -1.92311 | 2.201912 | -0.72149 |
| 14 | H | -1.75903 | 2.489406 | -1.63085 |
| 15 | H | -2.05703 | 3.004897 | -0.19808 |
| 16 | C | 0.960709 | -2.32625 | 1.715625 |
| 17 | O | 0.090918 | -3.18932 | 1.949934 |
| 18 | O | 0.738925 | -1.22686 | 1.079329 |
| 19 | C | 2.382194 | -2.55767 | 2.190673 |
| 20 | O | 2.522642 | -3.79777 | 2.862123 |
| 21 | H | 1.642709 | -4.20989 | 2.858979 |
| 22 | H | 3.047296 | -2.51744 | 1.313852 |
| 23 | H | 2.66003 | -1.72574 | 2.856826 |

**$[UO_2(H_2O)(glycolate)_2]^0$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.88396 | -0.01492 | 0.088201 |
| 2 | O | -0.29344 | -0.56277 | -1.50008 |
| 3 | O | -1.51045 | 0.503774 | 1.672307 |
| 4 | O | 1.138893 | 1.493026 | 0.390848 |
| 5 | O | -3.20462 | -0.1556 | -0.81678 |
| 6 | O | -1.85237 | -2.26925 | 0.53787 |
| 7 | H | 1.238864 | 2.269102 | -0.17758 |
| 8 | H | 2.017374 | 1.105617 | 0.506977 |
| 9 | H | -3.40927 | 0.714346 | -1.27863 |
| 10 | H | -3.93691 | -0.34288 | -0.21463 |
| 11 | H | -2.11938 | -2.82615 | -0.20543 |
| 12 | H | -1.17911 | -2.78877 | 1.075575 |
| 13 | C | 0.989386 | -2.32713 | 1.805196 |
| 14 | O | 0.139492 | -3.23713 | 1.923509 |
| 15 | O | 0.802094 | -1.22973 | 1.165021 |
| 16 | C | 2.349808 | -2.51263 | 2.455359 |
| 17 | O | 2.452861 | -3.76162 | 3.119667 |
| 18 | H | 1.592068 | -4.19723 | 2.998783 |

| | | | | |
|---|---|---|---|---|
| 19 | H | 3.120467 | -2.43018 | 1.67314 |
| 20 | H | 2.506227 | -1.68553 | 3.165716 |
| 21 | C | -2.22451 | 2.707554 | -1.53175 |
| 22 | O | -3.30959 | 2.214929 | -1.91144 |
| 23 | O | -1.34813 | 2.090335 | -0.82473 |
| 24 | C | -1.90001 | 4.140531 | -1.91806 |
| 25 | O | -2.93411 | 4.727547 | -2.69132 |
| 26 | H | -3.61713 | 4.04178 | -2.78352 |
| 27 | H | -1.73758 | 4.716857 | -0.99373 |
| 28 | H | -0.95342 | 4.140048 | -2.48088 |

**$[UO_2(glycolate)_3]^-$**

| Tag | Symbol | X | Y | Z |
|---|---|---|---|---|
| 1 | U | -1.39148 | -0.00023 | 0.06555 |
| 2 | O | -0.46978 | -0.59075 | -1.34739 |
| 3 | O | -2.30497 | 0.629839 | 1.468912 |
| 4 | O | 0.65282 | 1.269385 | 0.868319 |
| 5 | O | -3.38658 | 0.401884 | -1.43595 |
| 6 | H | 1.040761 | 1.900933 | 0.249812 |
| 7 | H | 1.356835 | 0.631365 | 1.172 |
| 8 | H | -3.52538 | 1.382859 | -1.5733 |
| 9 | H | -4.22147 | 0.004474 | -1.15842 |
| 10 | C | 1.094333 | -1.56797 | 1.907399 |
| 11 | O | 2.044124 | -0.75847 | 1.796717 |
| 12 | O | -0.10244 | -1.36119 | 1.502622 |
| 13 | C | 1.363506 | -2.90438 | 2.583677 |
| 14 | O | 2.715365 | -3.01897 | 3.002216 |
| 15 | H | 3.137348 | -2.18316 | 2.737435 |
| 16 | H | 0.686177 | -2.99856 | 3.446841 |
| 17 | H | 1.112893 | -3.70797 | 1.873778 |
| 18 | C | -2.8174 | -3.09284 | -0.36143 |
| 19 | O | -1.85041 | -3.796 | -0.68273 |
| 20 | O | -2.76931 | -1.87345 | 0.068401 |
| 21 | C | -4.21893 | -3.69151 | -0.45314 |
| 22 | O | -4.17031 | -5.03287 | -0.91757 |
| 23 | H | -3.22079 | -5.20436 | -1.05863 |
| 24 | H | -4.68726 | -3.64723 | 0.542693 |
| 25 | H | -4.82237 | -3.07119 | -1.13483 |
| 26 | C | -2.03099 | 3.137769 | -1.32693 |
| 27 | O | -3.2188 | 2.99808 | -1.70528 |
| 28 | O | -1.29356 | 2.210669 | -0.84698 |
| 29 | C | -1.39966 | 4.517584 | -1.45045 |
| 30 | O | -2.30263 | 5.462039 | -2.00619 |
| 31 | H | -3.12404 | 4.965747 | -2.16712 |
| 32 | H | -1.07669 | 4.840742 | -0.44838 |

| | | | | |
|---|---|---|---|---|
| 33 | H | -0.50007 | 4.432254 | -2.07986 |

**oxalate**

| | | | | |
|---|---|---|---|---|
| 1 | C | 2.498552 | -0.75811 | 0.030723 |
| 2 | C | 2.484778 | 0.782523 | -0.07351 |
| 3 | O | 1.660163 | 1.399074 | 0.66682 |
| 4 | O | 1.703213 | -1.38995 | -0.72843 |
| 5 | O | 3.301602 | -1.27179 | 0.866588 |
| 6 | O | 3.296668 | 1.311407 | -0.89111 |

**$[UO_2(H_2O)_3(oxalate)]^0$**

| Tag | Symbol | X | Y | Z |
|---|---|---|---|---|
| 1 | U | -0.56557 | 0.052363 | -0.00589 |
| 2 | O | -0.69315 | 0.141296 | 1.770931 |
| 3 | O | -0.59026 | -0.03413 | -1.7867 |
| 4 | O | -1.26891 | -2.39971 | 0.15953 |
| 5 | O | -3.06385 | 0.195172 | -0.12626 |
| 6 | O | -1.02776 | 2.557154 | -0.17755 |
| 7 | H | -0.50511 | -2.99549 | 0.139067 |
| 8 | H | -1.94089 | -2.79742 | -0.41156 |
| 9 | H | -3.6768 | 0.219934 | 0.621443 |
| 10 | H | -3.59771 | 0.195171 | -0.9325 |
| 11 | H | -1.71809 | 3.007092 | 0.329139 |
| 12 | H | -0.21747 | 3.075903 | -0.06436 |
| 13 | C | 2.532473 | -0.8425 | 0.09692 |
| 14 | C | 2.59145 | 0.719785 | 0.003066 |
| 15 | O | 1.405006 | 1.258936 | -0.0311 |
| 16 | O | 1.308338 | -1.2913 | 0.116166 |
| 17 | O | 3.548083 | -1.52281 | 0.143896 |
| 18 | O | 3.655283 | 1.322844 | -0.03179 |

**$[UO_2(H_2O)(oxalate)_2]^{2-}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | 0.033509 | -0.01038 | -0.07836 |
| 2 | O | 0.039705 | 0.067262 | -1.8766 |
| 3 | O | 0.020944 | -0.12189 | 1.717462 |
| 4 | O | -0.06249 | -2.5721 | -0.28537 |
| 5 | H | 0.664187 | -3.05623 | 0.129248 |
| 6 | H | -0.89877 | -2.92857 | 0.046195 |
| 7 | C | 3.143698 | 1.043665 | 0.006039 |
| 8 | C | 3.291989 | -0.51647 | -0.03379 |
| 9 | O | 2.158803 | -1.13434 | -0.08905 |
| 10 | O | 1.90965 | 1.433471 | -0.00297 |
| 11 | O | 4.130868 | 1.778686 | 0.041585 |
| 12 | O | 4.403991 | -1.04759 | -0.01135 |

| | | | | |
|---|---|---|---|---|
| 13 | C | -3.02323 | 1.197651 | 0.033016 |
| 14 | O | -1.76992 | 1.516828 | 0.007742 |
| 15 | C | -3.25872 | -0.34869 | -0.04905 |
| 16 | O | -3.96598 | 1.985516 | 0.112798 |
| 17 | O | -2.16157 | -1.02763 | -0.10896 |
| 18 | O | -4.4 | -0.81422 | -0.05227 |

**$[UO_2(oxalate)_3]^{4-}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | 0.587125 | 0.563403 | 0.041876 |
| 2 | O | 0.62489 | 0.8687 | 1.8232 |
| 3 | O | 0.541463 | 0.274669 | -1.74052 |
| 4 | O | 2.503715 | -4.26387 | 1.591669 |
| 5 | C | -2.6151 | 1.400569 | 0.002312 |
| 6 | O | -1.42776 | 1.884871 | -0.11696 |
| 7 | C | -2.63671 | -0.15219 | 0.218306 |
| 8 | O | -3.66939 | 2.045353 | -0.04036 |
| 9 | O | -1.46084 | -0.67622 | 0.280131 |
| 10 | O | -3.70685 | -0.76333 | 0.31249 |
| 11 | C | 2.508909 | 3.21506 | -0.43782 |
| 12 | O | 1.279197 | 2.839359 | -0.36523 |
| 13 | C | 3.531867 | 2.04542 | -0.22932 |
| 14 | O | 2.903884 | 4.367865 | -0.64823 |
| 15 | O | 2.968815 | 0.902667 | -0.03557 |
| 16 | O | 4.74929 | 2.256962 | -0.2572 |
| 17 | C | 1.649509 | -3.98022 | 0.70602 |
| 18 | C | 1.895193 | -2.67821 | -0.08087 |
| 19 | O | 0.625868 | -4.64447 | 0.382038 |
| 20 | O | 1.370341 | -1.61314 | 0.442914 |
| 21 | O | 2.566572 | -2.70843 | -1.12672 |

**$AHA^-$**

| | | | | |
|---|---|---|---|---|
| 1 | C | 0.947307 | 0.837227 | 0.030817 |
| 2 | O | 0.270526 | -0.21688 | 0.187707 |
| 3 | N | 2.278113 | 0.85768 | -0.10071 |
| 4 | H | 2.725525 | 1.762314 | -0.22424 |
| 5 | O | 3.098009 | -0.21801 | -0.08292 |
| 6 | C | 0.271704 | 2.196265 | -0.01993 |
| 7 | H | 0.979573 | 3.02177 | -0.1754 |
| 8 | H | -0.46691 | 2.209589 | -0.83439 |
| 9 | H | -0.27025 | 2.372414 | 0.920658 |

**$[UO_2(H_2O)_3(AHA)]^+$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -1.00189 | -0.24327 | -0.04946 |
| 2 | O | -1.10712 | -0.0483 | -1.81774 |
| 3 | O | -1.06938 | -0.3645 | 1.726372 |
| 4 | O | -3.506 | -0.04291 | 0.017585 |
| 5 | O | -1.8517 | -2.59178 | -0.22369 |
| 6 | H | -4.09927 | 0.009088 | -0.74373 |
| 7 | H | -4.05972 | -0.14177 | 0.803515 |
| 8 | H | -1.83933 | -3.0981 | -1.04769 |
| 9 | H | -1.77476 | -3.23366 | 0.495622 |
| 10 | O | -1.47953 | 2.203297 | 0.198708 |
| 11 | H | -1.34611 | 2.847012 | -0.5104 |
| 12 | H | -1.35927 | 2.68022 | 1.031198 |
| 13 | C | 2.197583 | 0.23037 | -0.04935 |
| 14 | O | 1.11773 | 0.906894 | 0.038026 |
| 15 | N | 2.086767 | -1.07818 | -0.17136 |
| 16 | H | 2.868934 | -1.71946 | -0.24678 |
| 17 | O | 0.842128 | -1.62681 | -0.19407 |
| 18 | C | 3.546955 | 0.873803 | -0.01562 |
| 19 | H | 4.353624 | 0.140695 | -0.12133 |
| 20 | H | 3.612825 | 1.608085 | -0.82899 |
| 21 | H | 3.663911 | 1.409572 | 0.93557 |

L-glycine$^-$

| | | | | |
|---|---|---|---|---|
| 1 | C | -1.41115 | -0.54979 | 1.750135 |
| 2 | O | -0.15183 | -0.59812 | 1.665169 |
| 3 | O | -2.11702 | 0.496049 | 1.866522 |
| 4 | C | -2.19566 | -1.88599 | 1.736967 |
| 5 | H | -2.68928 | -1.97744 | 2.717382 |
| 6 | H | -3.0028 | -1.80045 | 0.995667 |
| 7 | N | -1.43962 | -3.11611 | 1.473813 |
| 8 | H | -0.6037 | -3.10652 | 2.057434 |
| 9 | H | -1.07902 | -3.08357 | 0.521072 |

**$[UO_2(H_2O)_3(L\text{-glycine})]^+$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.99511 | 0.050906 | -0.01532 |
| 2 | O | -0.98579 | 0.068627 | -1.78316 |
| 3 | O | -1.04039 | 0.087066 | 1.751827 |
| 4 | O | 1.174095 | 1.208883 | 0.057877 |
| 5 | O | -3.42892 | -0.23926 | -0.11469 |
| 6 | H | 1.680592 | 1.413374 | 0.856197 |
| 7 | H | 1.737625 | 1.414216 | -0.70127 |
| 8 | H | -3.9529 | -0.35703 | -0.91914 |

| | | | | |
|---|---|---|---|---|
| 9 | H | -4.03208 | -0.31978 | 0.63744 |
| 10 | O | -1.79945 | 2.390408 | 0.03152 |
| 11 | H | -1.95172 | 2.963051 | -0.73324 |
| 12 | H | -1.97769 | 2.915043 | 0.824323 |
| 13 | C | -0.14699 | -2.65197 | 0.008057 |
| 14 | O | -1.38878 | -2.3918 | -0.00197 |
| 15 | O | 0.707839 | -1.71862 | 0.01098 |
| 16 | C | 0.328661 | -4.08807 | 0.020831 |
| 17 | H | 0.993174 | -4.27396 | -0.82826 |
| 18 | H | 0.870838 | -4.29451 | 0.949429 |
| 19 | N | -0.82982 | -5.02944 | -0.06686 |
| 20 | H | -1.34317 | -4.91821 | -0.94662 |
| 21 | H | -1.50021 | -4.87418 | 0.692518 |
| 22 | H | -0.51242 | -6.00198 | -0.01372 |

**Salicylate$^{2-}$**

| | | | | |
|---|---|---|---|---|
| 1 | C | -1.2716 | 0.307398 | 0.142709 |
| 2 | C | 0.114184 | 0.300676 | 0.323481 |
| 3 | C | 0.900018 | 1.501376 | 0.353241 |
| 4 | C | 0.158661 | 2.730193 | 0.176914 |
| 5 | C | -1.227 | 2.71207 | -0.00072 |
| 6 | C | -1.96495 | 1.51455 | -0.02152 |
| 7 | H | -1.81628 | -0.64078 | 0.129598 |
| 8 | H | 0.642155 | -0.64901 | 0.449732 |
| 9 | H | -1.75447 | 3.662545 | -0.12822 |
| 10 | H | -3.04683 | 1.529217 | -0.16136 |
| 11 | C | 0.894396 | 4.061308 | 0.186975 |
| 12 | O | 1.027491 | 4.646469 | 1.305027 |
| 13 | O | 1.308228 | 4.509762 | -0.92606 |
| 14 | O | 2.185462 | 1.480986 | 0.526486 |

**$[UO_2(H_2O)_3(Sal)]^0$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.66064 | -0.2808 | -0.03218 |
| 2 | O | -0.86825 | -0.00537 | -1.79322 |
| 3 | O | -0.66471 | -0.56797 | 1.739228 |
| 4 | O | -3.17991 | 0.014919 | 0.137046 |
| 5 | O | -1.71658 | -2.61627 | -0.3834 |
| 6 | H | -3.79727 | 0.074001 | -0.60428 |
| 7 | H | -3.7115 | -0.05603 | 0.941121 |
| 8 | H | -0.9902 | -3.25786 | -0.39179 |
| 9 | H | -2.39681 | -2.97989 | 0.199861 |
| 10 | O | -1.18182 | 2.19883 | 0.427191 |
| 11 | H | -1.96199 | 2.646991 | 0.073311 |
| 12 | H | -0.42847 | 2.78489 | 0.267937 |
| 13 | C | 4.840964 | 1.440596 | 0.181595 |

| | | | | |
|---|---|---|---|---|
| 14 | C | 3.462592 | 1.632072 | 0.195267 |
| 15 | C | 2.573675 | 0.546688 | 0.01965 |
| 16 | C | 3.110165 | -0.7574 | -0.17473 |
| 17 | C | 4.508896 | -0.91749 | -0.18489 |
| 18 | C | 5.376697 | 0.157445 | -0.00987 |
| 19 | H | 5.504053 | 2.295972 | 0.320683 |
| 20 | H | 3.036826 | 2.624794 | 0.342214 |
| 21 | H | 4.90138 | -1.92182 | -0.33632 |
| 22 | H | 6.455381 | 0.002985 | -0.02154 |
| 23 | C | 2.262793 | -1.98296 | -0.37628 |
| 24 | O | 2.788152 | -3.09263 | -0.53536 |
| 25 | O | 0.961373 | -1.83415 | -0.383 |
| 26 | O | 1.264594 | 0.791443 | 0.040888 |

Catecholate$^{2-}$

| | | | | |
|---|---|---|---|---|
| 1 | C | -2.17646 | 0.637925 | 0.018086 |
| 2 | C | -0.80851 | 0.597804 | 0.286366 |
| 3 | C | -0.08124 | 1.810044 | 0.341228 |
| 4 | C | -0.65993 | 3.091435 | 0.135406 |
| 5 | C | -2.11438 | 3.133467 | -0.15659 |
| 6 | C | -2.80008 | 1.889493 | -0.19659 |
| 7 | H | -2.76553 | -0.2824 | -0.03016 |
| 8 | H | -0.2979 | -0.35484 | 0.453934 |
| 9 | H | 0.993615 | 1.780657 | 0.555527 |
| 10 | H | -3.87537 | 1.922862 | -0.40868 |
| 11 | O | 0.049473 | 4.191166 | 0.200416 |
| 12 | O | -2.73047 | 4.270448 | -0.36551 |

**$[UO_2(H_2O)_3(Cat)]^0$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -1.00425 | -0.39291 | -0.07225 |
| 2 | O | -1.22598 | -0.31215 | -1.84986 |
| 3 | O | -0.98778 | -0.4284 | 1.72099 |
| 4 | O | -3.48157 | 0.26275 | 0.148317 |
| 5 | O | -1.40195 | -3.01089 | -0.20768 |
| 6 | H | -4.07488 | 0.521387 | -0.56888 |
| 7 | H | -3.96926 | 0.378953 | 0.974088 |
| 8 | H | -1.89449 | -3.39473 | -0.94544 |
| 9 | H | -0.4568 | -3.19069 | -0.37171 |
| 10 | O | -1.21639 | 2.177394 | -0.02612 |
| 11 | H | -0.26842 | 2.388716 | 0.047158 |
| 12 | H | -1.67158 | 2.649202 | 0.684131 |
| 13 | C | 4.500488 | -1.33879 | -0.42542 |
| 14 | C | 4.562232 | 0.055963 | -0.41113 |
| 15 | C | 3.380778 | 0.820814 | -0.32935 |
| 16 | C | 2.142987 | 0.176837 | -0.26259 |

| | | | | |
|---|---|---|---|---|
| 17 | C | 2.081092 | -1.24472 | -0.27945 |
| 18 | C | 3.255362 | -1.99612 | -0.35971 |
| 19 | H | 5.416883 | -1.92742 | -0.48795 |
| 20 | H | 5.527575 | 0.561454 | -0.46354 |
| 21 | H | 3.421227 | 1.911198 | -0.31816 |
| 22 | H | 3.196824 | -3.08571 | -0.37059 |
| 23 | O | 0.952831 | 0.802668 | -0.18282 |
| 24 | O | 0.839837 | -1.76255 | -0.21297 |

**Formate$^{-}$**

| | | | | |
|---|---|---|---|---|
| 1 | C | -1.08615 | -0.82622 | 0.305065 |
| 2 | H | -2.10611 | -0.5787 | -0.10074 |
| 3 | O | -0.55793 | 0.049913 | 1.041833 |
| 4 | O | -0.61536 | -1.94565 | -0.03414 |

**$[UO_2(H_2O)_4(Formate)]^{+}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -1.00907 | -0.14317 | 0.137179 |
| 2 | O | -0.8706 | -0.43323 | -1.60537 |
| 3 | O | -1.25474 | 0.133012 | 1.871116 |
| 4 | O | 0.732252 | 1.607196 | 0.005427 |
| 5 | O | -3.51623 | -0.01524 | -0.11832 |
| 6 | O | -1.79097 | -2.47861 | 0.400019 |
| 7 | H | 0.797348 | 2.273119 | 0.703964 |
| 8 | H | 1.629977 | 1.141047 | -0.04232 |
| 9 | H | -3.98679 | -0.38167 | -0.88051 |
| 10 | H | -4.12123 | -0.07704 | 0.634597 |
| 11 | H | -1.80468 | -3.14965 | -0.29584 |
| 12 | H | -1.98016 | -2.92699 | 1.235548 |
| 13 | O | -1.87333 | 2.191731 | -0.3513 |
| 14 | H | -1.35376 | 2.791087 | -0.90514 |
| 15 | H | -2.80007 | 2.293758 | -0.60979 |
| 16 | C | 2.267894 | -1.0217 | 0.292827 |
| 17 | H | 2.888816 | -1.92094 | 0.450359 |
| 18 | O | 2.804226 | 0.049137 | -0.03744 |
| 19 | O | 1.00276 | -1.1864 | 0.483048 |

**[Nicotinate]$^-$**

| | | | | |
|---|---|---|---|---|
| 1 | C | -0.66462 | 0.832281 | -0.27868 |
| 2 | C | 0.200059 | 1.926584 | -0.36891 |
| 3 | C | -1.45767 | 3.384959 | 0.259018 |
| 4 | C | -2.41052 | 2.362661 | 0.381856 |
| 5 | C | -3.85101 | 2.668466 | 0.804217 |
| 6 | C | -1.98871 | 1.056958 | 0.10244 |
| 7 | N | -0.17952 | 3.188394 | -0.10652 |
| 8 | O | -4.12994 | 3.878731 | 1.037324 |
| 9 | O | -4.63792 | 1.683406 | 0.883443 |
| 10 | H | -1.75493 | 4.412791 | 0.469012 |
| 11 | H | 1.242073 | 1.783742 | -0.66457 |
| 12 | H | -0.30193 | -0.17092 | -0.50342 |
| 13 | H | -2.70068 | 0.237133 | 0.186733 |

**$[UO_2(H_2O)_3(Nicotinate)]^{2+}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.79786 | -0.01119 | -0.22309 |
| 2 | O | -0.88245 | 0.500209 | -1.91427 |
| 3 | O | -0.71852 | -0.45175 | 1.488761 |
| 4 | O | 1.300373 | 1.251349 | -0.00677 |
| 5 | O | -3.23069 | -0.39486 | -0.33327 |
| 6 | H | 1.879616 | 1.272958 | 0.767728 |
| 7 | H | 1.765099 | 1.700271 | -0.72649 |
| 8 | H | -3.77602 | -0.34458 | -1.13061 |
| 9 | H | -3.78759 | -0.74652 | 0.375241 |
| 10 | O | -1.61166 | 2.251857 | 0.373207 |
| 11 | H | -1.83383 | 2.95571 | -0.25176 |
| 12 | H | -1.77209 | 2.595408 | 1.263139 |
| 13 | C | 0.390259 | -6.23835 | -1.89547 |
| 14 | C | 1.766528 | -6.39457 | -1.93205 |
| 15 | C | 2.088848 | -4.11584 | -1.34753 |
| 16 | C | 0.715307 | -3.91423 | -1.29738 |
| 17 | C | 0.187126 | -2.56129 | -0.94519 |
| 18 | C | -0.14228 | -4.9877 | -1.57377 |
| 19 | N | 2.560865 | -5.33613 | -1.65878 |
| 20 | O | 0.992222 | -1.60107 | -0.72995 |
| 21 | O | -1.0646 | -2.3685 | -0.8546 |
| 22 | H | 2.815078 | -3.33416 | -1.14583 |
| 23 | H | 2.265874 | -7.32962 | -2.17035 |
| 24 | H | -0.25095 | -7.08806 | -2.11529 |
| 25 | H | -1.21943 | -4.83694 | -1.53514 |
| 26 | H | 3.569675 | -5.46779 | -1.68844 |

**$[UO_2(H_2O)_4(Nicotinate)]^{2+}$**

| | | | | |
|---|---|---|---|---|
| 1 | U | -0.91454 | 0.008932 | -0.00198 |
| 2 | O | -0.88365 | -0.21838 | -1.75749 |
| 3 | O | -1.02149 | 0.208224 | 1.753803 |
| 4 | O | 0.636564 | 1.917051 | -0.23188 |
| 5 | O | -3.42226 | -0.16007 | 0.059762 |
| 6 | O | -1.38696 | -2.39948 | 0.27838 |
| 7 | H | 0.687642 | 2.591954 | 0.459155 |
| 8 | H | 1.568304 | 1.5557 | -0.36226 |
| 9 | H | -3.95954 | -0.51597 | -0.66232 |
| 10 | H | -3.91323 | -0.3203 | 0.878048 |
| 11 | H | -1.45611 | -3.05419 | -0.42976 |
| 12 | H | -1.54897 | -2.85927 | 1.113361 |
| 13 | O | -2.05783 | 2.24518 | -0.31701 |
| 14 | H | -1.7044 | 2.904374 | -0.9307 |
| 15 | H | -3.02194 | 2.271032 | -0.39472 |
| 16 | C | 4.05319 | -3.93859 | 0.661533 |
| 17 | C | 5.375316 | -3.63893 | 0.378438 |
| 18 | C | 4.791873 | -1.40971 | -0.19573 |
| 19 | C | 3.453257 | -1.66332 | 0.076291 |
| 20 | C | 2.451542 | -0.55168 | -0.09883 |
| 21 | C | 3.083223 | -2.94401 | 0.507706 |
| 22 | N | 5.695275 | -2.39399 | -0.03873 |
| 23 | O | 2.850422 | 0.570566 | -0.45966 |
| 24 | O | 1.227798 | -0.85456 | 0.153628 |
| 25 | H | 5.15517 | -0.44421 | -0.53433 |
| 26 | H | 6.193009 | -4.34844 | 0.468706 |
| 27 | H | 3.791108 | -4.93884 | 0.997113 |
| 28 | H | 2.037261 | -3.15438 | 0.721815 |
| 29 | H | 6.670665 | -2.18802 | -0.24384 |