

**Supporting Information for Non-Covalent Interactions of Uranyl Complexes: A Theoretical Study, Platts and Baker**

**Cartesian coordinates of [UO<sub>2</sub>Cl<sub>2</sub>(H<sub>2</sub>O)<sub>3</sub>]**

|    |           |           |           |
|----|-----------|-----------|-----------|
| U  | -0.005343 | 0.029822  | -0.004040 |
| O  | 0.172896  | 0.171510  | 1.774077  |
| O  | -0.271399 | 0.078705  | -1.772667 |
| Cl | 2.627824  | 0.314015  | -0.303639 |
| O  | 0.915942  | -2.342050 | 0.048740  |
| O  | 0.544032  | 2.560241  | -0.058473 |
| Cl | -2.088920 | -1.622058 | 0.363187  |
| O  | -2.166303 | 1.444023  | 0.167054  |
| H  | 0.278716  | -2.890048 | 0.547549  |
| H  | 1.778875  | -2.391535 | 0.500251  |
| H  | 1.507865  | 2.429445  | -0.217339 |
| H  | 0.477246  | 2.920241  | 0.845298  |
| H  | -2.751760 | 0.679152  | 0.374872  |
| H  | -2.430373 | 1.736649  | -0.724812 |

**Cartesian coordinates of [UO<sub>2</sub>(NCSe)<sub>2</sub>(H<sub>2</sub>O)<sub>3</sub>]**

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | 0.136019  | 0.168401  | 1.792562  |
| U  | -0.020620 | 0.024208  | 0.004038  |
| O  | -2.180456 | 1.456838  | 0.157589  |
| O  | -0.263568 | 0.088013  | -1.775465 |
| N  | 2.320514  | 0.209171  | -0.244738 |
| O  | 0.954319  | -2.343291 | 0.050949  |
| O  | 0.541867  | 2.563552  | -0.055906 |
| N  | -1.805898 | -1.495727 | 0.295020  |
| H  | 0.392691  | -2.944153 | 0.574031  |
| H  | 1.851703  | -2.377901 | 0.429355  |
| H  | 1.467791  | 2.582331  | -0.368422 |
| H  | 0.570546  | 2.909161  | 0.855091  |
| H  | -2.855716 | 0.865579  | 0.543021  |
| H  | -2.496969 | 1.661301  | -0.741557 |
| C  | -2.760079 | -2.202113 | 0.447905  |
| Se | -4.164499 | -3.231853 | 0.675622  |
| C  | 3.503913  | 0.340067  | -0.367925 |
| Se | 5.240042  | 0.538333  | -0.544390 |

### Cartesian coordinates of $[\text{UO}_2\text{Cl}_2(\text{H}_2\text{O})_3]\dots\text{H}_2\text{O}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | -0.079204 | -0.529479 | -0.675130 |
| U  | 1.618316  | -0.189758 | -0.136313 |
| O  | 1.056108  | 2.332901  | -0.359508 |
| O  | 3.221822  | 0.324155  | 0.469045  |
| Cl | 1.552433  | -2.275352 | 1.457833  |
| O  | 2.503809  | -2.129011 | -1.513213 |
| O  | 0.620115  | 0.770918  | 1.952377  |
| Cl | 2.194251  | 0.701672  | -2.619225 |
| H  | 2.349550  | -1.908941 | -2.453141 |
| H  | 2.038559  | -2.960609 | -1.307126 |
| H  | 0.786831  | 0.121335  | 2.661921  |
| H  | -0.383313 | 0.781187  | 1.795959  |
| H  | 1.415878  | 2.397464  | -1.276770 |
| H  | 1.665513  | 2.836670  | 0.210485  |
| H  | -1.569275 | 0.161229  | 0.337242  |
| O  | -1.880406 | 0.682631  | 1.115156  |
| H  | -2.159577 | 1.537527  | 0.743547  |

### Cartesian coordinates of $[\text{UO}_2\text{Cl}_2(\text{H}_2\text{O})_3]\dots\text{Br}-\text{Cl}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| U  | -0.100643 | -0.303613 | -0.771073 |
| Cl | 2.341984  | 0.390827  | -0.075108 |
| Cl | -2.613946 | 0.476995  | -1.161532 |
| O  | -0.464432 | -0.908302 | 0.871709  |
| O  | 0.281413  | 0.104214  | -2.505028 |
| O  | 1.328912  | -2.379399 | -1.151142 |
| O  | -1.450653 | -2.305084 | -1.647522 |
| O  | -0.217944 | 2.149524  | -0.165540 |
| H  | 1.537562  | -2.377203 | -2.117512 |
| H  | 2.168470  | -2.138072 | -0.707694 |
| H  | -1.564664 | -2.988048 | -0.961431 |
| H  | -2.317898 | -1.848278 | -1.728752 |
| H  | -0.934903 | 2.585931  | -0.664092 |
| H  | 0.621478  | 2.604867  | -0.365277 |
| Br | 1.531185  | -1.240257 | -4.231967 |
| Cl | 2.645490  | -2.577499 | -5.618464 |