**SUPPORTING INFORMATION**

**Uranium separation from acid mine drainage using anionic resins – An experimental /theoretical investigation of its chemical speciation and the interaction mechanism.**

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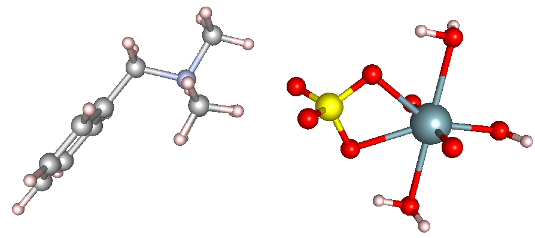
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**Figure S1:** Coefficient of linear correlation between estimated ΔG(aq) of hydrolysis species and log β.

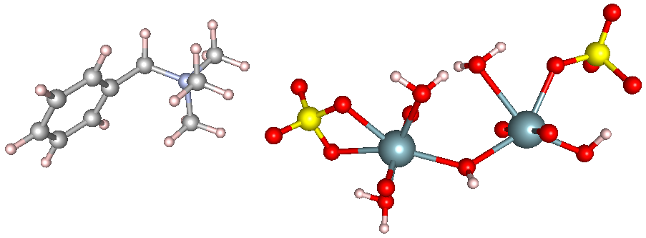
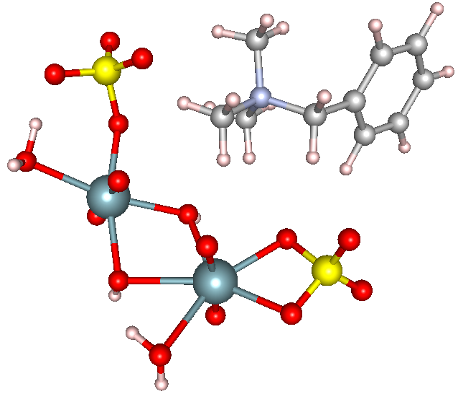


**Figure S2:** Most stable optimized structures at the B3LYP/SDD level of theory:

a) [UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)] b)[(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)] e c) [(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]-.



**(a)**

**(b) (c)**

**Table S3:** Estimated ΔG(aq) and ΔG(g) for the interaction between the lowest energy uranium species, the sulfate and the benzyltrimethylammonium group, obtained from the thermodynamic cycle, calculated at the B3LYP/SDD level of theory.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Complexes** | | **Reactions** | **ΔG(g)**  **(Kcal mol-1)** | **ΔG(aq)**  **(Kcal mol-1)** |
| A | [UO2OH(H2O)4]+(aq) + SO42-(aq) + Ar-CH2N+(CH3)3  [UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)](aq) + 2H2O | | -183.21 | 129.92 | |
| B | [(UO2)2(OH)(H2O)8]3+(aq) + 2SO42-(aq) + Ar-CH2N+(CH3)3  [(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)](aq) + 4H2O | | -692.81 | 124.78 | |
| C | [(UO2)2(OH)2(H2O)6]2+(aq)+ 2SO42-(aq) + Ar-CH2N+(CH3)3  [(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]-(aq) + 4H2O | | -493.63 | 129.01 | |
| D | [UO2OH(H2O)4]+(aq) + [SO4(Ar-CH2N(CH3)3)]-(aq)  [UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)](aq) +2H2O | | -133.20 | -16.71 | |
| E | [(UO2)2(OH)(H2O)8]3+(aq) + SO42-(aq) + [SO4(Ar-CH2N(CH3)3)]-(aq)[(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)](aq) + 4H2O | | -642.81 | -21.86 | |
| F | [(UO2)2(OH)2(H2O)6]2+(aq)+ SO42-(aq) + [SO4(Ar-CH2N(CH3)3)]-(aq)[(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]-(aq) + 4H2O | | -443.63 | -17.62 | |
| G | SO42-(aq) + Ar-CH2N+(CH3)3[SO4(Ar-CH2N(CH3)3)]-(aq) | | -50.01 | 139.48 | |

**Table S4:** Estimated ΔG(aq) and ΔG(g) for the interaction between the lowest energy uranium-sulfate species and the benzyltrimethylammonium group, obtained from the thermodynamic cycle, calculated at the B3LYP/SDD level of theory.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Complexes** | | **Reactions** | **ΔG(g)**  **(Kcal mol-1)** | **ΔG(aq)**  **(Kcal mol-1)** |
| A | [UO2SO4(H2O)4](aq) + Ar-CH2N+(CH3)3 [UO2SO4(H2O)4(Ar-CH2N(CH3)3)]+(aq) | | -73.49 | -50.40 | |
| B | [UO2(SO4)2(H2O)]2-(aq) + Ar-CH2N+(CH3)3[UO2(SO4)2(H2O)(Ar-CH2N(CH3)3)]-(aq) | | -149.34 | -33.74 | |
| C | SO42-(aq) + Ar-CH2N+(CH3)3[SO4(Ar-CH2N(CH3)3)]-(aq) | | -50.01 | 139.48 | |

**Table S5:** Calculated gas phase ΔG(g) (Electronic Energy, *Eelet*, more Thermal Correction Energy, *Etherm*), and the solvation energy,ΔG(solv) of the different chemical species. Thermal corrections estimated at 298.15 K and 1 atm.

|  |  |  |
| --- | --- | --- |
| **Species** | **ΔG(g) (*Eelet* + *Etherm*)(Hartree)** | **ΔG(solv) (Kcal mol-1)** |
| [UO2(H2O)5]2+ | -583.580082 | -225.49 |
| H2O | -76.416024 | -7.86 |
| H3O+ | -76.688265 | -76.19 |
| [UO2OH(H2O)4]+ | -583.350183 | -87.58 |
| [(UO2)2(OH)(H2O)8]3+ | -1090.372774 | -398.12 |
| [(UO2)2(OH)2(H2O)6]2+ | -1013.800581 | -220.44 |
| SO42- | -698.944242 | -246.69 |
| [UO2SO4(H2O)4] | -1206.766921 | -58.34 |
| [UO2(SO4)2(H2O)]2- | -1676.658505 | -187.00 |
| Ar-CH2N+(CH3)3 | -445.239958 | -51.69 |
| [SO4(Ar-CH2N(CH3)3)]- | -1144.263891 | -101.74 |
| [UO2SO4(H2O)4(Ar-CH2N(CH3)3)]+ | -1651.820680 | -86.93 |
| [UO2(SO4)2(H2O)(Ar-CH2N(CH3)3)]- | -2121.885506 | -123.08 |
| [UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)] | -1574.994300 | -57.11 |
| [(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)] | -2628.941188 | -94.16 |
| [(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]- | -2552.051577 | -111.43 |

**S6:** Cartesian coordinates of optimized geometries for hydrolysis reaction of the ion [UO2(H2O)5]2+.

**H2O**

**Total energy in Hartrees**

scf done B3LYP/ 6-31g(d,p): -76.423014

**Optimized coordinates (in Angstroms) at the B3LYP/6-31g(d,p) level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.000000 | 0.000000 | 0.119188 |
| H | 0.000000 | 0.759286 | -0.476754 |
| H | 0.000000 | -0.759286 | -0.476754 |

**H3O+**

**Total energy in Hartrees**

scf done B3LYP/ 6-31g(d,p): -76.810436

**Optimized coordinates (in Angstroms) at the B3LYP/6-31g(d,p) level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.000000 | 0.000000 | 0.000000 |
| H | 0.000000 | 0.976459 | 0.000000 |
| H | 0.845638 | -0.488229 | 0.000000 |
| H | -0.845638 | -0.488229 | 0.000000 |

**[UO2(H2O)5]2+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -583.860629

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.408651 | -0.317684 | -1.650474 |
| O | -0.180374 | 0.450464 | 1.683541 |
| O | 2.230962 | -0.855927 | 0.568009 |
| O | -1.062266 | 2.142119 | -0.743755 |
| O | -1.251666 | -2.146603 | -0.565969 |
| H | -0.671281 | 2.699155 | -1.432086 |
| H | -2.023520 | 2.129132 | -0.866269 |
| H | 2.617323 | -0.906309 | 1.454509 |
| H | 2.811619 | -1.344881 | -0.033262 |
| H | -0.926278 | -2.665045 | -1.316609 |
| H | -1.522775 | -2.780735 | 0.115412 |
| O | -2.569503 | 0.224294 | 0.336961 |
| H | -3.138616 | -0.415748 | -0.116468 |
| O | 1.603366 | 1.884562 | -0.284120 |
| H | 2.335309 | 1.806010 | -0.914173 |
| H | 1.923539 | 2.426005 | 0.452869 |
| H | -2.904845 | 0.305127 | 1.242136 |
| U | -0.007984 | 0.011785 | 0.007584 |

**[UO2OH(H2O)4]+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -583.439756

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 2.816703 | -0.298297 | -1.707004 |
| O | 2.705330 | 0.453673 | 1.733117 |
| O | 5.103215 | -0.922068 | 0.135486 |
| O | 1.760714 | 2.359946 | -0.447580 |
| O | 2.261771 | -2.012161 | 0.511267 |
| H | 2.394926 | 2.959680 | -0.867306 |
| H | 0.950538 | 2.376487 | -0.977226 |
| H | 5.469061 | -1.130081 | 1.008025 |
| H | 5.274387 | -1.700847 | -0.414448 |
| H | 2.111414 | -2.362616 | 1.399644 |
| O | 0.196940 | 0.091234 | -0.304885 |
| H | -0.153648 | -0.567698 | -0.922356 |
| O | 4.455198 | 1.920515 | -0.344291 |
| H | 5.143368 | 1.754045 | -1.005428 |
| H | 4.914088 | 2.282937 | 0.428140 |
| H | -0.355591 | 0.026152 | 0.488503 |
| U | 2.735567 | 0.017477 | 0.026476 |

**[UO2(OH)2(H2O)3]**

**Total energy in Hartrees**

scf done B3LYP/SDD: -582.995542

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 3.018416 | -0.172040 | -1.770828 |
| O | 2.415092 | 0.199988 | 1.706657 |
| O | 5.035970 | -1.126220 | 0.385470 |
| O | 1.873702 | 2.490359 | -0.581941 |
| O | 2.600830 | -2.222946 | 0.217323 |
| H | 2.038655 | 2.776774 | -1.491882 |
| H | 1.020649 | 1.993412 | -0.610968 |
| H | 5.678921 | -1.138341 | -0.337708 |
| H | 4.549465 | -1.974739 | 0.335940 |
| H | 2.297406 | -2.585278 | 1.060633 |
| O | 0.491822 | 0.263786 | -0.384153 |
| O | 4.517645 | 1.811976 | 0.258847 |
| H | 5.245706 | 1.863904 | -0.376470 |
| H | 4.068372 | 2.669804 | 0.215370 |
| H | -0.095906 | 0.214349 | 0.381857 |
| U | 2.677996 | -0.025043 | -0.032426 |

**[UO2(OH)3(H2O)2]-**

**Total energy in Hartrees**

scf done B3LYP/SDD: -582.549784

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 2.894899 | -0.647721 | -1.572959 |
| O | 2.957449 | -0.563870 | 2.022057 |
| O | 4.984362 | -1.465534 | 0.188885 |
| O | 2.006881 | 2.954855 | -0.841243 |
| O | 1.816329 | -2.554943 | 0.297094 |
| H | 1.941291 | 2.880517 | -1.802897 |
| H | 1.506103 | 2.161729 | -0.481880 |
| H | 5.320469 | -1.697412 | -0.687100 |
| H | 1.651465 | -2.966407 | -0.561332 |
| O | 1.078687 | 0.732677 | 0.223168 |
| O | 4.107812 | 1.681711 | 0.105050 |
| H | 4.878454 | 1.685326 | -0.478486 |
| H | 3.427543 | 2.287723 | -0.315162 |
| H | 0.748467 | 0.932088 | 1.109754 |
| U | 2.926601 | -0.629112 | 0.224769 |

**[(UO2)2(OH)(H2O)8]3+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -1090.876282

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -1.744575 | 0.679001 | -1.307844 |
| O | -2.788896 | -0.519224 | 1.799249 |
| O | -0.117844 | -0.447293 | 0.807022 |
| O | -4.154337 | 1.734145 | 0.366905 |
| O | -2.151456 | -2.025680 | -1.344165 |
| H | -4.074271 | 2.603267 | -0.052535 |
| H | -2.140477 | -2.943573 | -1.035802 |
| O | -4.717669 | -0.994897 | -0.094872 |
| O | -1.505353 | 2.132141 | 1.165242 |
| H | -0.548152 | 2.309385 | 1.009692 |
| H | -5.027391 | -1.621484 | 0.575139 |
| U | -2.328232 | 0.008861 | 0.197251 |
| H | -1.687543 | 2.339210 | 2.093580 |
| H | -5.045399 | 1.401756 | 0.177579 |
| H | -5.017452 | -1.334145 | -0.951223 |
| H | -1.585907 | -1.982280 | -2.128643 |
| O | 1.204110 | 2.338187 | 0.598061 |
| H | 1.702954 | 2.686515 | 1.354676 |
| O | 2.969027 | 1.637286 | -1.636149 |
| H | 3.793891 | 2.109117 | -1.446434 |
| O | 4.343069 | -0.898361 | -0.641353 |
| H | 5.026543 | -1.099142 | 0.014908 |
| O | 2.058469 | -2.592561 | 0.384716 |
| H | 2.481322 | -3.008267 | 1.150435 |
| H | 1.923888 | -3.281770 | -0.282295 |
| H | 2.950116 | 1.481187 | -2.591606 |
| H | 1.354995 | 2.962503 | -0.130800 |
| H | 4.610062 | -1.316131 | -1.473440 |
| O | 2.610083 | 0.041118 | 1.543121 |
| O | 1.468905 | -0.638126 | -1.675384 |
| H | -0.078653 | -0.676789 | 1.748893 |
| U | 2.029050 | -0.182088 | -0.087981 |

**[(UO2)2(OH)2(H2O)6]2+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -1014.033883

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -1.642799 | 0.018610 | -1.361404 |
| O | -1.552277 | -0.808823 | 2.042064 |
| O | 0.146054 | 1.127550 | 0.721601 |
| O | -4.117572 | -0.331942 | 1.290876 |
| H | -4.211659 | -0.083094 | 2.221518 |
| O | -3.190839 | -2.279598 | -0.355410 |
| O | -2.625919 | 2.050568 | 0.134892 |
| H | -3.077536 | 2.263072 | -0.694087 |
| H | -3.748882 | -2.622113 | 0.358394 |
| U | -1.641210 | -0.346184 | 0.351446 |
| H | -3.092645 | 2.525987 | 0.836537 |
| H | -4.857391 | 0.079875 | 0.821811 |
| H | -2.852068 | -3.046022 | -0.841415 |
| O | 2.712613 | 2.441383 | 1.028071 |
| H | 3.484458 | 2.520227 | 1.607849 |
| O | 4.284123 | 1.065662 | -1.294198 |
| H | 5.135963 | 1.277420 | -0.886926 |
| O | 3.343594 | -1.836061 | -0.976257 |
| H | 3.930628 | -2.378076 | -0.429473 |
| O | 0.441828 | -1.412815 | -0.034133 |
| H | 4.158922 | 1.688650 | -2.023698 |
| H | 2.673722 | 3.260047 | 0.511696 |
| H | 3.702310 | -1.856772 | -1.875404 |
| O | 2.634172 | -0.400997 | 1.520783 |
| O | 1.629056 | 0.697662 | -1.653933 |
| H | 0.195928 | 1.538089 | 1.597464 |
| H | 0.614887 | -2.133176 | 0.591081 |
| U | 2.151516 | 0.188195 | -0.061237 |

**[(UO2)3(OH)4(H2O)7]2+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -1444.209926

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -3.405706 | -0.103612 | -1.855591 |
| O | -4.015057 | 0.520332 | 1.545723 |
| O | -2.158241 | 1.906918 | -0.238589 |
| O | -6.310891 | -0.470766 | 0.313174 |
| H | -6.731566 | 0.029309 | 1.027313 |
| O | -4.253321 | -2.240453 | 0.156193 |
| O | -5.127854 | 2.027134 | -1.456662 |
| H | -5.368615 | 1.846692 | -2.376067 |
| H | -5.075186 | -2.369876 | 0.653702 |
| U | -3.754819 | 0.240016 | -0.170075 |
| H | -5.825488 | 2.586941 | -1.087762 |
| H | -6.964403 | -0.522843 | -0.399307 |
| H | -3.595371 | -2.854297 | 0.511670 |
| O | 0.155311 | 3.516754 | 0.236626 |
| H | 0.858185 | 3.748133 | 0.860701 |
| O | 2.334890 | 1.512118 | -0.612571 |
| O | 1.477747 | -1.011672 | -0.039649 |
| O | -1.677952 | -0.723281 | 0.300799 |
| H | 2.451190 | 1.880880 | -1.501036 |
| H | 0.276670 | 4.103286 | -0.524329 |
| H | 1.254818 | -1.712680 | -0.669930 |
| O | 0.248817 | 1.095275 | 1.539481 |
| O | -0.166412 | 0.597538 | -1.923391 |
| H | -2.213856 | 2.629605 | 0.404191 |
| H | -1.575572 | -1.011524 | 1.220362 |
| U | 0.031492 | 0.893343 | -0.196876 |
| O | 5.149519 | 1.752092 | -0.544848 |
| H | 6.070499 | 1.654699 | -0.259741 |
| O | 3.611348 | 0.094261 | 1.614652 |
| O | 6.240401 | -0.674599 | 0.147162 |
| H | 6.709742 | -1.216204 | -0.504501 |
| O | 3.958602 | -2.751029 | 0.423475 |
| H | 4.259130 | -3.423294 | -0.204294 |
| O | 3.873766 | -0.754407 | -1.782300 |
| H | 4.832999 | 2.601363 | -0.204809 |
| H | 6.619761 | -0.900989 | 1.009358 |
| H | 4.045106 | -3.129698 | 1.310039 |
| U | 3.699175 | -0.303331 | -0.094201 |

**[(UO2)3(OH)5(H2O)5]+**

**Total energy in Hartrees**

scf done B3LYP/SDD: -1367.448211

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -3.629976 | -0.038186 | -1.655202 |
| O | -3.944543 | 0.109659 | 1.832402 |
| O | -2.179119 | 1.790003 | 0.181343 |
| O | -6.317790 | -0.086631 | -0.028739 |
| H | -6.773346 | -0.733019 | -0.585499 |
| O | -4.386311 | -2.423121 | -0.006803 |
| O | -4.816561 | 2.385092 | -0.292847 |
| H | -5.462514 | 2.529230 | -0.997871 |
| H | -4.396747 | -2.970865 | 0.790931 |
| U | -3.713677 | 0.081506 | 0.091871 |
| H | -4.035655 | 2.925396 | -0.494355 |
| H | -6.857552 | 0.034621 | 0.764976 |
| H | -3.899976 | -2.923693 | -0.678800 |
| O | 0.291341 | 3.353407 | -0.206522 |
| H | 1.258964 | 3.274072 | -0.324980 |
| O | 2.250840 | 1.593931 | -0.740169 |
| O | 1.494558 | -1.097136 | -0.326572 |
| O | -1.679389 | -0.943903 | 0.284152 |
| H | 2.388880 | 1.688292 | -1.694857 |
| H | -0.041662 | 3.854212 | -0.963181 |
| H | 1.479660 | -1.459599 | -1.225425 |
| O | 0.371071 | 0.833175 | 1.509769 |
| O | -0.273735 | 0.660634 | -1.938624 |
| H | -2.068805 | 2.253588 | 1.025688 |
| H | -1.430281 | -1.323251 | 1.139732 |
| U | 0.079501 | 0.736055 | -0.216684 |
| O | 5.349420 | 1.905514 | -0.550371 |
| H | 6.183297 | 1.419116 | -0.427887 |
| O | 3.584174 | 0.352228 | 1.607367 |
| O | 5.909750 | -0.673513 | 0.397440 |
| O | 3.609093 | -2.616029 | 0.687743 |
| H | 4.176579 | -3.277671 | 0.270014 |
| O | 4.013254 | -0.633216 | -1.747907 |
| H | 5.344901 | 2.605270 | 0.117142 |
| H | 6.290233 | -0.744864 | 1.282613 |
| H | 2.686245 | -2.818177 | 0.467183 |
| U | 3.854580 | -0.161635 | -0.052846 |

**[(UO2)3(OH)7(H2O)]-**

**Total energy in Hartrees**

scf done B3LYP/SDD: -1213.621659

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -3.535594 | -0.043969 | -1.941827 |
| O | -4.222500 | 0.558142 | 1.484242 |
| O | -1.848875 | 1.557145 | -0.096710 |
| O | -6.052978 | 0.295151 | -0.641380 |
| H | -6.691439 | 0.386371 | 0.078885 |
| O | -4.623262 | -2.173855 | -0.041149 |
| H | -3.827995 | -2.702299 | -0.209506 |
| O | -3.909209 | 0.292056 | -0.240484 |
| H | -5.289160 | -2.449693 | -0.686990 |
| O | 2.101108 | 0.912752 | -0.123755 |
| O | 1.442873 | -1.782807 | 0.426000 |
| O | -2.095468 | -1.184071 | 0.414128 |
| H | 2.278685 | 1.187667 | -1.035109 |
| H | 1.422155 | -2.405309 | -0.315642 |
| O | 0.020309 | 0.316942 | 1.859787 |
| O | -0.151717 | -0.367919 | -1.616210 |
| H | -1.864647 | 2.157973 | 0.663135 |
| H | -2.197439 | -1.422803 | 1.347734 |
| U | -0.054772 | -0.010791 | 0.118078 |
| O | 3.442551 | -0.353394 | 2.251926 |
| O | 5.393143 | 0.639979 | 0.404147 |
| O | 4.827231 | -2.619442 | 1.188651 |
| O | 3.945228 | -1.251251 | -1.179121 |
| H | 5.623343 | 1.108661 | 1.217383 |
| H | 4.963976 | -2.713670 | 2.140719 |
| U | 3.723395 | -0.806999 | 0.544050 |

**S7:** Cartesian coordinates of optimized geometries of reaction of ion [UO2(H2O)5]2+ in sulfated medium.

**SO42-**

**Total energy in Hartrees**

scf done B3LYP/ 6-31g(d,p): -246.69

**Optimized coordinates (in Angstroms) at the B3LYP/6-31g(d,p) level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -0.694731 | 1.356189 | -0.067171 |
| S | 0.000015 | 0.000022 | -0.000002 |
| O | 1.469613 | 0.162331 | -0.374928 |
| O | -0.104902 | -0.555347 | 1.416626 |
| O | -0.670010 | -0.963217 | -0.974523 |

**[UO2SO4(H2O)4]**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1206.941328

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.196699 | -0.113802 | -1.914761 |
| O | 0.012179 | 0.261014 | 1.560555 |
| O | 2.042450 | -1.395196 | 0.153669 |
| O | -0.926245 | 2.498173 | 0.070963 |
| O | -0.903597 | -2.176570 | 0.443503 |
| H | -1.714225 | 2.216216 | 0.680273 |
| H | -1.374440 | 2.803199 | -0.731659 |
| H | 1.993903 | -1.850336 | 1.007135 |
| H | 2.272135 | -2.064334 | -0.504979 |
| H | -1.294380 | -2.669291 | -0.292321 |
| H | -1.721323 | -1.823984 | 0.968446 |
| O | -2.195063 | 0.105977 | -0.556390 |
| O | 1.738780 | 1.979172 | -0.225192 |
| H | 2.126494 | 2.283679 | -1.056132 |
| H | 1.139790 | 2.683936 | 0.083789 |
| S | -3.267342 | 0.194282 | 0.676448 |
| O | -4.608454 | 0.157081 | 0.106011 |
| O | -2.902123 | -1.001835 | 1.519516 |
| O | -2.897552 | 1.495250 | 1.344006 |
| U | -0.042035 | 0.089217 | -0.178846 |

**[UO2SO4(H2O)3]**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1130.485339

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -0.409872 | 0.108208 | -1.722367 |
| O | 0.412529 | 0.099116 | 1.574030 |
| O | -1.405776 | 2.524407 | -0.064832 |
| O | -0.879485 | -2.365403 | 0.136345 |
| H | -2.318978 | 2.436591 | 0.334610 |
| H | -1.582532 | 2.751607 | -0.988875 |
| H | -1.695739 | -2.462809 | -0.381595 |
| H | -1.108567 | -2.636506 | 1.038222 |
| O | -2.695778 | -0.115126 | -0.599071 |
| O | 1.663756 | 1.545953 | -0.429853 |
| H | 1.808894 | 2.055382 | -1.237166 |
| H | 2.059973 | 2.032767 | 0.305044 |
| S | -3.395733 | 0.241518 | 0.767877 |
| O | -3.840156 | 1.658089 | 0.715737 |
| O | -4.367128 | -0.768933 | 1.162661 |
| O | -2.088513 | 0.184811 | 1.658146 |
| U | -0.461528 | 0.148547 | 0.042359 |

**[UO2(SO4)2(H2O)3]2-**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1829.868510

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.069905 | -0.181684 | -1.069757 |
| O | -0.930886 | 0.408843 | 2.265035 |
| O | 1.486253 | -0.724537 | 1.740605 |
| O | -1.182854 | 2.423469 | 0.110415 |
| O | -0.418193 | -2.477460 | 0.706378 |
| H | -2.239549 | 2.349652 | 0.179994 |
| H | -0.981261 | 2.584191 | -0.819937 |
| H | 0.569441 | -2.606825 | 0.474251 |
| H | -0.442943 | -2.656274 | 1.656232 |
| O | -2.594997 | -0.084415 | -0.009456 |
| O | 1.653299 | 1.676019 | 0.372228 |
| H | 2.320867 | 0.939463 | 0.173035 |
| H | 1.832063 | 1.872625 | 1.301722 |
| S | -4.012139 | 0.654448 | 0.070262 |
| O | -4.670914 | 0.465009 | -1.241724 |
| O | -4.750901 | 0.101919 | 1.225647 |
| O | -3.637624 | 2.124399 | 0.294957 |
| S | 2.716083 | -1.410146 | 1.039077 |
| O | 3.690139 | -1.825378 | 2.071806 |
| O | 3.281106 | -0.369646 | 0.093638 |
| O | 2.139371 | -2.592969 | 0.280308 |
| U | -0.448654 | 0.084796 | 0.596452 |

**[UO2(SO4)2(H2O)2]2-**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1753.425471

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| U | -0.005516 | -0.043080 | 0.464947 |
| O | 0.270922 | 0.090900 | 2.205736 |
| O | -0.302292 | -0.179416 | -1.273683 |
| O | 2.041217 | -1.218700 | 0.168374 |
| O | 1.991080 | 1.167593 | -0.005873 |
| O | -1.068598 | 2.259324 | -0.163453 |
| H | -1.980739 | 1.880156 | -0.394904 |
| H | -0.633521 | 2.366391 | -1.020309 |
| H | -0.551874 | -2.669263 | -0.641713 |
| O | -0.985577 | -2.450444 | 0.194298 |
| H | -1.912616 | -2.144029 | -0.082694 |
| O | -2.246421 | -0.033610 | 1.093433 |
| S | -3.479110 | -0.130775 | 0.116493 |
| O | -3.300049 | -1.447249 | -0.614330 |
| O | -4.729978 | -0.087854 | 0.903386 |
| O | -3.339862 | 1.058086 | -0.814259 |
| S | 3.009842 | -0.019820 | -0.128178 |
| O | 4.044509 | 0.077812 | 0.922161 |
| O | 3.533670 | -0.110069 | -1.507791 |

**[UO2(SO4)2(H2O)]2-**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1130.485339

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | -0.409872 | 0.108208 | -1.722367 |
| O | 0.412529 | 0.099116 | 1.574030 |
| O | -1.405776 | 2.524407 | -0.064832 |
| O | -0.879485 | -2.365403 | 0.136345 |
| H | -2.318978 | 2.436591 | 0.334610 |
| H | -1.582532 | 2.751607 | -0.988875 |
| H | -1.695739 | -2.462809 | -0.381595 |
| H | -1.108567 | -2.636506 | 1.038222 |
| O | -2.695778 | -0.115126 | -0.599071 |
| O | 1.663756 | 1.545953 | -0.429853 |
| H | 1.808894 | 2.055382 | -1.237166 |
| H | 2.059973 | 2.032767 | 0.305044 |
| S | -3.395733 | 0.241518 | 0.767877 |
| O | -3.840156 | 1.658089 | 0.715737 |
| O | -4.367128 | -0.768933 | 1.162661 |
| O | -2.088513 | 0.184811 | 1.658146 |
| U | -0.461528 | 0.148547 | 0.042359 |

**S8:** Cartesian coordinates of optimized geometries for interaction of species with ion exchange resin.

**(Ar-CH2N+(CH3)3)**

**Total energy in Hartrees**

scf done B3LYP/ 6-31g(d,p): -445.508761

**Optimized coordinates (in Angstroms) at the B3LYP/6-31g(d,p) level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| N | -3.405197 | -0.000061 | 0.099559 |
| C | -2.604488 | 1.201908 | -0.109568 |
| H | -2.315590 | 1.346544 | -1.170649 |
| H | -3.173871 | 2.085622 | 0.206394 |
| H | -1.685112 | 1.124511 | 0.482603 |
| C | -2.606004 | -1.201779 | -0.116737 |
| H | -3.176472 | -2.086618 | 0.194087 |
| H | -2.317476 | -1.340498 | -1.178710 |
| H | -1.686409 | -1.129040 | 0.475749 |
| C | -4.606506 | 0.003178 | -0.708507 |
| H | -4.406128 | 0.006298 | -1.802153 |
| H | -5.211766 | -0.884694 | -0.486808 |
| H | -5.210561 | 0.890541 | -0.481533 |
| C | 0.451767 | -0.008527 | 1.778663 |
| H | 0.150715 | 0.913545 | 2.271850 |
| H | 0.153075 | -0.934774 | 2.265415 |
| C | 1.505894 | -0.004005 | 0.862843 |
| C | 2.103346 | -1.210907 | 0.334997 |
| C | 2.100216 | 1.208027 | 0.343270 |
| C | 3.134093 | -1.195095 | -0.589255 |
| H | 1.715262 | -2.167998 | 0.685128 |
| C | 3.130987 | 1.201208 | -0.581063 |
| H | 1.709681 | 2.161699 | 0.699949 |
| C | 3.680703 | 0.005453 | -1.078423 |
| H | 3.533495 | -2.148349 | -0.942749 |
| H | 3.527915 | 2.157889 | -0.928023 |
| H | 4.489576 | 0.008983 | -1.804788 |

**[UO2SO4(H2O)4(Ar-CH2N(CH3)3)]+**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1572.640942

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.022680 | 0.769454 | 0.898598 |
| S | -0.727470 | 0.275076 | -0.273816 |
| O | -1.542751 | -1.013356 | 0.103581 |
| O | -1.947443 | 1.214257 | -0.577368 |
| O | 0.080749 | 0.050901 | -1.479224 |
| N | 3.573973 | 1.195419 | 0.281215 |
| C | 3.229245 | 0.730815 | -1.111345 |
| H | 2.157972 | 0.522605 | -1.167886 |
| H | 3.496071 | 1.522520 | -1.813441 |
| H | 3.804799 | -0.167054 | -1.331109 |
| C | 3.193772 | 0.122859 | 1.269460 |
| H | 3.470249 | 0.459710 | 2.269952 |
| H | 2.113750 | -0.020766 | 1.210811 |
| H | 3.732540 | -0.790384 | 1.022185 |
| C | 2.776915 | 2.437751 | 0.593127 |
| H | 1.717072 | 2.178477 | 0.573803 |
| H | 3.058062 | 2.791153 | 1.586343 |
| H | 3.010976 | 3.199181 | -0.151946 |
| C | 5.072055 | 1.546793 | 0.390267 |
| H | 5.219963 | 2.371662 | -0.310930 |
| H | 5.198826 | 1.932140 | 1.404802 |
| C | 6.033041 | 0.421016 | 0.114637 |
| C | 6.491931 | -0.395838 | 1.159596 |
| C | 6.529560 | 0.208944 | -1.180887 |
| C | 7.403845 | -1.420865 | 0.909546 |
| H | 6.148598 | -0.220340 | 2.175851 |
| C | 7.441677 | -0.815775 | -1.431360 |
| H | 6.214234 | 0.856656 | -1.994728 |
| C | 7.875571 | -1.635052 | -0.387171 |
| H | 7.753945 | -2.043048 | 1.727134 |
| H | 7.820719 | -0.966743 | -2.437158 |
| H | 8.590135 | -2.428939 | -0.580914 |
| O | -3.862867 | -0.705892 | -1.858845 |
| O | -3.885725 | 0.259356 | 1.502298 |
| O | -4.683355 | 2.052945 | -0.849207 |
| O | -3.567930 | -2.700889 | 0.470270 |
| H | -4.325044 | 2.353436 | -1.698300 |
| H | -4.482174 | 2.756469 | -0.214106 |
| H | -3.739724 | -3.368806 | -0.208287 |
| H | -2.613940 | -2.748850 | 0.659942 |
| O | -6.206075 | -0.821442 | -0.001894 |
| H | -6.817552 | -1.012335 | -0.725646 |
| H | -6.720879 | -0.775369 | 0.815258 |
| U | -3.728498 | -0.218872 | -0.177356 |

**[UO2(SO4)2(H2O)(Ar-CH2N(CH3)3)]-**

**Total energy in Hartrees**

scf done B3LYP/ SDD: =-2122.1364572

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| U | 2.54263 | -0.00280 | 0.10546 |
| O | 2.80103 | 1.59017 | 0.82751 |
| O | 2.25140 | -1.63785 | -0.52428 |
| O | 4.73553 | -0.68816 | 0.79041 |
| O | 4.35440 | 0.27934 | -1.36279 |
| O | 0.66048 | 0.75238 | -1.11548 |
| H | 2.14148 | -2.29333 | 1.75903 |
| O | 1.98742 | -1.51825 | 2.31773 |
| H | 1.08431 | -1.21094 | 2.06611 |
| O | 0.25987 | -0.01114 | 1.11608 |
| S | -0.53641 | 0.48362 | -0.14114 |
| O | -1.24225 | 1.74390 | 0.16706 |
| O | -1.39889 | -0.59960 | -0.66007 |
| S | 5.53300 | -0.31128 | -0.50155 |
| O | 6.53067 | 0.74021 | -0.21317 |
| O | 6.08027 | -1.52260 | -1.14878 |
| N | -4.80524 | 1.08500 | 0.07760 |
| C | -4.48379 | 0.25809 | 1.29695 |
| H | -3.40534 | 0.08812 | 1.34415 |
| H | -4.81736 | 0.80494 | 2.18047 |
| H | -5.01675 | -0.68880 | 1.22569 |
| C | -4.33337 | 0.35553 | -1.15397 |
| H | -4.59323 | 0.95133 | -2.03054 |
| H | -3.24978 | 0.24718 | -1.08606 |
| H | -4.82974 | -0.61236 | -1.20144 |
| C | -4.06683 | 2.39742 | 0.16873 |
| H | -2.99573 | 2.18867 | 0.16529 |
| H | -4.33251 | 3.00680 | -0.69642 |
| H | -4.36754 | 2.90443 | 1.08646 |
| C | -6.31561 | 1.38889 | -0.00010 |
| H | -6.53229 | 1.97280 | 0.89771 |
| H | -6.42823 | 2.04149 | -0.86916 |
| C | -7.22270 | 0.19146 | -0.10097 |
| C | -7.60017 | -0.31266 | -1.35523 |
| C | -7.75118 | -0.40174 | 1.05606 |
| C | -8.46291 | -1.40423 | -1.44973 |
| H | -7.23217 | 0.15946 | -2.26249 |
| C | -8.61415 | -1.49315 | 0.96204 |
| H | -7.49981 | 0.00013 | 2.03413 |
| C | -8.96658 | -1.99874 | -0.29096 |
| H | -8.75025 | -1.78206 | -2.42586 |
| H | -9.01877 | -1.94031 | 1.86449 |
| H | -9.64304 | -2.84455 | -0.36448 |

**[UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)]**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -1572.124726

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 0.084765 | 0.796646 | 0.811142 |
| S | -0.715731 | 0.305272 | -0.352934 |
| O | -1.417256 | -1.022739 | 0.005121 |
| O | -1.922366 | 1.235657 | -0.595579 |
| O | 0.109760 | 0.161638 | -1.576291 |
| N | 3.459681 | 1.177379 | 0.162605 |
| C | 3.137313 | 0.574216 | -1.182428 |
| H | 2.056934 | 0.389890 | -1.248456 |
| H | 3.441997 | 1.283384 | -1.954666 |
| H | 3.699248 | -0.352781 | -1.288815 |
| C | 3.071271 | 0.202635 | 1.246886 |
| H | 3.337777 | 0.639249 | 2.211454 |
| H | 1.987937 | 0.059076 | 1.187320 |
| H | 3.616268 | -0.727580 | 1.093300 |
| C | 2.640803 | 2.434748 | 0.338180 |
| H | 1.585569 | 2.145064 | 0.360653 |
| H | 2.925621 | 2.901164 | 1.283078 |
| H | 2.858389 | 3.108302 | -0.492002 |
| C | 4.942534 | 1.557096 | 0.259009 |
| H | 5.094449 | 2.316020 | -0.512631 |
| H | 5.053496 | 2.036406 | 1.234757 |
| C | 5.928127 | 0.427485 | 0.102534 |
| C | 6.381918 | -0.282964 | 1.223991 |
| C | 6.447759 | 0.102766 | -1.159507 |
| C | 7.312154 | -1.312588 | 1.083846 |
| H | 6.013747 | -0.023682 | 2.213098 |
| C | 7.378157 | -0.926527 | -1.301087 |
| H | 6.129806 | 0.663017 | -2.034693 |
| C | 7.807875 | -1.638894 | -0.179880 |
| H | 7.654276 | -1.853452 | 1.960769 |
| H | 7.771354 | -1.166531 | -2.284104 |
| H | 8.534300 | -2.438400 | -0.289150 |
| O | -3.894357 | -0.723619 | -1.842784 |
| O | -3.740518 | 0.066793 | 1.600169 |
| O | -4.343583 | 2.217691 | -0.386422 |
| O | -3.277532 | -2.863820 | 0.142300 |
| H | -3.391068 | 2.432422 | -0.429924 |
| H | -4.649499 | 2.514118 | 0.481554 |
| H | -3.479721 | -3.268559 | -0.712223 |
| H | -2.320398 | -2.662491 | 0.116139 |
| O | -5.947534 | -0.614368 | -0.005811 |
| H | -6.450109 | -0.815771 | -0.805387 |
| U | -3.811235 | -0.319017 | -0.122635 |

**[(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)]**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -2623.369055

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| O | 3.836774 | -0.347372 | -1.546253 |
| O | 6.172865 | -1.184800 | -0.204109 |
| O | 2.122623 | -1.546056 | 0.577723 |
| H | 2.152739 | -2.012573 | 1.425569 |
| O | 0.565618 | 0.181709 | -1.131044 |
| U | 4.197742 | -0.332875 | 0.174876 |
| O | 4.410218 | -0.426026 | 1.919578 |
| U | -0.075614 | -0.966804 | 0.043307 |
| O | 0.456864 | 0.803715 | 1.789888 |
| H | 1.187942 | 1.371307 | 1.470289 |
| O | -0.219242 | -2.848403 | -1.714254 |
| O | -0.593021 | -2.162503 | 1.224294 |
| O | 7.495979 | 1.106179 | 0.691372 |
| S | 6.664962 | 2.174087 | -0.209373 |
| O | 5.175518 | 1.775300 | 0.103926 |
| O | 6.955848 | 3.482749 | 0.352825 |
| O | 6.943101 | 1.904454 | -1.620530 |
| O | -4.167266 | -0.529573 | 0.147270 |
| S | -2.954922 | 0.025432 | -0.511064 |
| O | -1.920334 | 0.480232 | 0.555945 |
| O | -2.146806 | -1.112299 | -1.196080 |
| O | -3.255521 | 1.116127 | -1.460880 |
| H | 6.461842 | -1.323114 | -1.116849 |
| H | 7.230336 | 0.196544 | 0.400187 |
| H | -0.317291 | -3.735071 | -1.341392 |
| H | -1.098380 | -2.594509 | -2.051274 |
| N | -7.103746 | 1.281594 | -0.582269 |
| C | -6.661913 | 1.225107 | 0.858873 |
| H | -5.655220 | 0.800344 | 0.881898 |
| H | -6.678533 | 2.237530 | 1.265917 |
| H | -7.352525 | 0.588123 | 1.409863 |
| C | -6.998295 | -0.102038 | -1.172894 |
| H | -7.244012 | -0.044499 | -2.234519 |
| H | -5.974390 | -0.450398 | -1.018876 |
| H | -7.702958 | -0.753972 | -0.658452 |
| C | -6.181238 | 2.206036 | -1.341017 |
| H | -5.156448 | 1.820774 | -1.299435 |
| H | -6.520237 | 2.253485 | -2.377256 |
| H | -6.239969 | 3.197244 | -0.888345 |
| C | -8.532474 | 1.835961 | -0.707846 |
| H | -8.477108 | 2.854739 | -0.316652 |
| H | -8.720999 | 1.893443 | -1.782555 |
| C | -9.614663 | 1.050493 | -0.013790 |
| C | -10.316162 | 0.045299 | -0.697157 |
| C | -9.976650 | 1.348984 | 1.308648 |
| C | -11.335401 | -0.664873 | -0.063352 |
| H | -10.072932 | -0.175520 | -1.733254 |
| C | -10.995473 | 0.639135 | 1.943480 |
| H | -9.467191 | 2.147730 | 1.841299 |
| C | -11.672669 | -0.372262 | 1.259489 |
| H | -11.870487 | -1.439031 | -0.604450 |
| H | -11.265086 | 0.881273 | 2.966717 |
| H | -12.468395 | -0.922798 | 1.751817 |
| H | -0.355594 | 1.335112 | 1.786011 |
| O | 2.541333 | 1.788869 | 0.251581 |
| H | 2.119529 | 1.779377 | -0.623377 |
| H | 3.328440 | 2.371995 | 0.200543 |

**[(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]-**

**Total energy in Hartrees**

scf done B3LYP/ SDD: -2546.506266

**Optimized coordinates (in Angstroms) at the B3LYP/SDD level of theory.**

**X Y Z**

|  |  |  |  |
| --- | --- | --- | --- |
| N | 1.7539700 | 2.5723410 | 1.0270420 |
| C | 1.6653650 | 4.0647230 | 1.1682520 |
| H | 0.6220240 | 4.3482270 | 1.0103870 |
| H | 1.9929440 | 4.3404900 | 2.1730140 |
| H | 2.3132050 | 4.5293200 | 0.4255720 |
| C | 1.2581820 | 2.1926320 | -0.3461540 |
| H | 1.3309060 | 1.1125720 | -0.4614740 |
| H | 0.2226200 | 2.5241670 | -0.4210760 |
| H | 1.8805940 | 2.6949940 | -1.0862880 |
| C | 0.8471280 | 1.9435350 | 2.0585190 |
| H | -0.1612420 | 2.3279500 | 1.8964580 |
| H | 0.8696980 | 0.8619660 | 1.9351090 |
| H | 1.2192410 | 2.2202230 | 3.0474570 |
| C | 3.1795640 | 2.0503140 | 1.2671520 |
| H | 3.4280730 | 2.3667430 | 2.2841410 |
| H | 3.1210290 | 0.9577670 | 1.2464020 |
| C | 4.2159090 | 2.5351960 | 0.2844480 |
| C | 4.5212390 | 1.7600960 | -0.8449340 |
| C | 4.9295610 | 3.7223960 | 0.5070080 |
| C | 5.4990170 | 2.1845560 | -1.7452840 |
| H | 4.0030960 | 0.8192920 | -1.0025190 |
| C | 5.9067640 | 4.1460590 | -0.3940000 |
| H | 4.7304370 | 4.3122990 | 1.3987110 |
| C | 6.1889670 | 3.3783760 | -1.5256930 |
| H | 5.7286020 | 1.5708830 | -2.6112090 |
| H | 6.4519390 | 5.0672830 | -0.2077400 |
| H | 6.9532270 | 3.7033460 | -2.2264990 |
| O | -1.9968810 | 0.3672330 | 1.3143890 |
| O | -4.7404630 | 0.9703360 | 0.6989420 |
| O | -2.2270980 | -2.2909570 | 0.1509160 |
| H | -2.5113800 | -2.7327170 | -0.6631900 |
| O | 0.4000310 | -1.3435630 | 1.5398160 |
| U | -2.6339870 | 0.0334050 | -0.2943400 |
| O | -3.3413260 | -0.4513740 | -1.8463960 |
| U | 0.4409050 | -2.2928240 | 0.0574740 |
| O | -0.4829910 | -0.4339890 | -1.1093350 |
| H | -0.4085700 | -0.5084070 | -2.0700700 |
| O | -0.8491540 | -4.1638900 | 1.3742530 |
| O | 0.2874550 | -3.3115980 | -1.3832010 |
| O | -3.9411570 | 3.3533710 | 0.7150210 |
| S | -2.6751420 | 3.5655010 | -0.0956770 |
| O | -2.4839580 | 2.1593420 | -0.8641260 |
| O | -2.8104920 | 4.6049280 | -1.1233220 |
| O | -1.4788060 | 3.7204960 | 0.7851130 |
| O | 4.4197920 | -2.5427570 | -0.9051370 |
| S | 3.4680090 | -1.9803720 | 0.0581300 |
| O | 2.3577800 | -1.1327530 | -0.6772450 |
| O | 2.5362000 | -3.1043760 | 0.6461520 |
| O | 4.0440930 | -1.1577470 | 1.1429520 |
| H | -4.7722670 | 0.7885250 | 1.6480590 |
| H | -4.4873000 | 1.9900520 | 0.6652860 |
| H | -1.6459580 | -3.6262420 | 1.1178670 |
| H | -0.8954470 | -4.9795970 | 0.8585130 |

**S9:** Vibrational analysis.

**[UO2(H2O)5]2+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 63.9195 | 92.8918 | 93.9014 |
| Frequencies | 111.1540 | 117.7468 | 136.4628 |
| Frequencies | 153.7096 | 160.3155 | 171.9407 |
| Frequencies | 183.9519 | 206.9977 | 210.0463 |
| Frequencies | 228.3207 | 244.9998 | 250.4791 |
| Frequencies | 266.3705 | 271.4911 | 287.2013 |
| Frequencies | 299.3118 | 308.8329 | 315.5052 |
| Frequencies | 338.2836 | 348.7247 | 352.3898 |
| Frequencies | 369.5309 | 391.6476 | 514.4187 |
| Frequencies | 521.3911 | 538.3275 | 568.8058 |
| Frequencies | 583.1089 | 918.3247 | 977.4705 |
| Frequencies | 1581.2951 | 1622.7111 | 1625.8622 |
| Frequencies | 1628.9727 | 1632.1604 | 3772.6478 |
| Frequencies | 3775.8964 | 3778.6964 | 3779.4534 |
| Frequencies | 3785.0719 | 3870.7849 | 3873.0108 |
| Frequencies | 3874.6531 | 3879.8886 | 3880.2622 |

**[UO2OH(H2O)4]+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 66.6120 | 69.9677 | 74.6856 |
| Frequencies | 87.1602 | 98.0115 | 105.9726 |
| Frequencies | 122.4246 | 132.1506 | 159.5580 |
| Frequencies | 170.3186 | 189.9801 | 195.1809 |
| Frequencies | 228.7114 | 235.0458 | 251.9521 |
| Frequencies | 256.1210 | 266.0691 | 272.9486 |
| Frequencies | 280.3408 | 356.6477 | 386.9306 |
| Frequencies | 389.4013 | 413.4599 | 414.4096 |
| Frequencies | 451.2935 | 526.5853 | 532.5033 |
| Frequencies | 536.3389 | 543.3391 | 548.5065 |
| Frequencies | 880.1559 | 931.6873 | 1584.1928 |
| Frequencies | 1634.5046 | 1637.9060 | 1638.9149 |
| Frequencies | 3777.6770 | 3783.1333 | 3783.9738 |
| Frequencies | 3785.2320 | 3840.8664 | 3872.0899 |
| Frequencies | 3874.4682 | 3874.6170 | 3881.0150 |

**[UO2(OH)2(H2O)3]**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 52.4827 | 65.5783 | 86.0381 |
| Frequencies | 105.5527 | 111.6774 | 150.4394 |
| Frequencies | 170.3036 | 182.9311 | 188.3094 |
| Frequencies | 192.3881 | 218.7005 | 231.9189 |
| Frequencies | 241.3592 | 252.6096 | 257.8188 |
| Frequencies | 300.8149 | 333.5840 | 377.5103 |
| Frequencies | 413.8555 | 430.2015 | 443.4688 |
| Frequencies | 465.1344 | 476.1883 | 525.8610 |
| Frequencies | 538.3513 | 544.3172 | 547.7695 |
| Frequencies | 665.0371 | 761.9782 | 857.5896 |
| Frequencies | 903.6585 | 1606.1326 | 1626.8515 |
| Frequencies | 1640.9131 | 3428.4317 | 3599.6733 |
| Frequencies | 3779.0552 | 3834.0967 | 3837.8247 |
| Frequencies | 3839.1377 | 3845.7417 | 3876.7120 |

**[UO2(OH)3(H2O)2]-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 37.8550 | 80.5934 | 91.4446 |
| Frequencies | 101.5496 | 127.9154 | 144.0286 |
| Frequencies | 189.2414 | 194.9378 | 231.1836 |
| Frequencies | 252.4320 | 258.0081 | 280.5085 |
| Frequencies | 299.7220 | 337.4830 | 337.7939 |
| Frequencies | 364.0786 | 378.4341 | 394.3781 |
| Frequencies | 417.9640 | 433.0753 | 465.1411 |
| Frequencies | 508.0799 | 536.0727 | 546.3553 |
| Frequencies | 610.8365 | 670.8607 | 811.5529 |
| Frequencies | 859.6879 | 869.9586 | 1067.465 |
| Frequencies | 1664.2644 | 1688.5926 | 3020.826 |
| Frequencies | 3167.0497 | 3834.5055 | 3836.935 |
| Frequencies | 3839.3402 | 3845.3147 | 3850.204 |

**[(UO2)2(OH)(H2O)8]3+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 33.0720 | 45.0265 | 63.8272 |
| Frequencies | 69.9962 | 76.442 | 81.3712 |
| Frequencies | 86.2836 | 91.0393 | 106.9524 |
| Frequencies | 121.0931 | 126.3189 | 128.5873 |
| Frequencies | 140.7167 | 146.8305 | 149.9713 |
| Frequencies | 154.8801 | 159.4808 | 172.7756 |
| Frequencies | 177.8404 | 191.5037 | 198.591 |
| Frequencies | 206.7661 | 214.0978 | 222.7934 |
| Frequencies | 228.6795 | 230.6622 | 236.1111 |
| Frequencies | 243.5700 | 245.3984 | 248.9871 |
| Frequencies | 256.9222 | 261.6634 | 265.4688 |
| Frequencies | 274.5457 | 275.4143 | 289.1001 |
| Frequencies | 293.9042 | 296.7992 | 308.2099 |
| Frequencies | 309.4282 | 312.3243 | 316.2917 |
| Frequencies | 320.7526 | 330.6135 | 342.0713 |
| Frequencies | 371.5111 | 371.8923 | 394.1965 |
| Frequencies | 412.4557 | 454.3342 | 502.8993 |
| Frequencies | 511.3055 | 512.978 | 517.611 |
| Frequencies | 532.7110 | 538.6354 | 551.9472 |
| Frequencies | 554.2749 | 652.1948 | 760.7481 |
| Frequencies | 890.5049 | 904.1704 | 913.3334 |
| Frequencies | 965.5633 | 973.6319 | 1604.252 |
| Frequencies | 1622.4860 | 1625.499 | 1626.464 |
| Frequencies | 1627.3152 | 1632.472 | 1633.015 |
| Frequencies | 1664.2349 | 3460.507 | 3754.314 |
| Frequencies | 3774.0914 | 3781.194 | 3782.923 |
| Frequencies | 3784.6341 | 3785.864 | 3786.567 |
| Frequencies | 3794.6596 | 3832.969 | 3842.754 |
| Frequencies | 3873.0815 | 3875.365 | 3877.4 |
| Frequencies | 3878.2770 | 3881.296 | 3884.214 |

**[(UO2)2(OH)2(H2O)6]2+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 50.5191 | 61.3949 | 66.8792 |
| Frequencies | 80.7575 | 82.3119 | 89.77 |
| Frequencies | 97.6365 | 100.5839 | 122.3139 |
| Frequencies | 131.4365 | 136.2922 | 143.2198 |
| Frequencies | 152.882 | 155.5151 | 163.5688 |
| Frequencies | 167.0683 | 170.321 | 173.2734 |
| Frequencies | 179.7797 | 197.7436 | 200.1657 |
| Frequencies | 213.8394 | 229.4512 | 234.5067 |
| Frequencies | 235.4406 | 237.8208 | 248.5217 |
| Frequencies | 251.702 | 263.0083 | 264.0133 |
| Frequencies | 270.1928 | 277.9156 | 289.586 |
| Frequencies | 290.2382 | 298.7862 | 300.5385 |
| Frequencies | 306.5544 | 321.8255 | 346.3873 |
| Frequencies | 354.0144 | 369.565 | 388.0273 |
| Frequencies | 395.0708 | 403.1813 | 434.164 |
| Frequencies | 481.1472 | 492.8058 | 507.058 |
| Frequencies | 515.6503 | 519.039 | 521.8601 |
| Frequencies | 539.4282 | 747.8016 | 788.9499 |
| Frequencies | 889.7296 | 897.0122 | 949.9676 |
| Frequencies | 954.9178 | 1605.042 | 1618.694 |
| Frequencies | 1619.365 | 1626.06 | 1630.42 |
| Frequencies | 1632.656 | 3777.655 | 3783.305 |
| Frequencies | 3787.508 | 3789.417 | 3791.675 |
| Frequencies | 3792.853 | 3811.827 | 3818.679 |
| Frequencies | 3876.309 | 3877.99 | 3881.431 |
| Frequencies | 3887.485 | 3890.964 | 3891.591 |

**[(UO2)3(OH)4(H2O)7]2+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 8.5352 | 30.5763 | 38.6884 |
| Frequencies | 49.3581 | 52.6861 | 65.8934 |
| Frequencies | 66.4529 | 70.7428 | 74.818 |
| Frequencies | 82.2352 | 90.0599 | 98.449 |
| Frequencies | 102.8488 | 107.6591 | 110.7102 |
| Frequencies | 116.0751 | 121.2625 | 123.0728 |
| Frequencies | 135.5767 | 145.7618 | 152.6201 |
| Frequencies | 155.5253 | 159.0263 | 170.6901 |
| Frequencies | 174.8352 | 175.8705 | 178.5055 |
| Frequencies | 189.1115 | 193.3184 | 209.8017 |
| Frequencies | 210.4585 | 211.9994 | 218.874 |
| Frequencies | 227.0557 | 230.6206 | 239.9873 |
| Frequencies | 244.6758 | 249.2706 | 250.0553 |
| Frequencies | 252.8899 | 262.0547 | 266.4765 |
| Frequencies | 274.6814 | 276.6656 | 279.7534 |
| Frequencies | 281.719 | 284.3969 | 288.2651 |
| Frequencies | 294.3526 | 296.2055 | 303.3531 |
| Frequencies | 324.9432 | 339.1845 | 348.4292 |
| Frequencies | 363.9801 | 366.074 | 374.7144 |
| Frequencies | 379.6469 | 389.9651 | 395.4764 |
| Frequencies | 410.0782 | 427.1444 | 431.3632 |
| Frequencies | 457.7306 | 465.9248 | 470.5175 |
| Frequencies | 479.0104 | 485.6804 | 493.7546 |
| Frequencies | 498.4535 | 503.5825 | 531.8147 |
| Frequencies | 537.5246 | 719.3681 | 735.5333 |
| Frequencies | 763.8769 | 785.7493 | 872.8398 |
| Frequencies | 891.7148 | 894.0707 | 932.0337 |
| Frequencies | 946.2777 | 952.2886 | 1584.101 |
| Frequencies | 1594.937 | 1615.959 | 1621.881 |
| Frequencies | 1624.443 | 1627.3 | 1629.65 |
| Frequencies | 3774.514 | 3776.844 | 3782.577 |
| Frequencies | 3786.835 | 3789.837 | 3792.155 |
| Frequencies | 3793.442 | 3810.622 | 3811.414 |
| Frequencies | 3816.169 | 3819.067 | 3873.934 |
| Frequencies | 3878.313 | 3880.308 | 3883.827 |
| Frequencies | 3885.43 | 3888.142 | 3893.055 |

**[(UO2)3(OH)5(H2O)5]+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 18.8375 | 23.1773 | 27.5576 |
| Frequencies | 36.4365 | 47.4739 | 51.0587 |
| Frequencies | 54.4583 | 58.7609 | 61.6094 |
| Frequencies | 68.7748 | 73.7753 | 76.5691 |
| Frequencies | 80.6916 | 97.6316 | 101.8461 |
| Frequencies | 111.8918 | 114.4054 | 119.5665 |
| Frequencies | 124.0944 | 130.0005 | 135.2479 |
| Frequencies | 143.5595 | 155.8489 | 167.5596 |
| Frequencies | 180.1437 | 190.9492 | 198.7852 |
| Frequencies | 214.4419 | 216.4576 | 219.82 |
| Frequencies | 225.7882 | 227.8617 | 231.0979 |
| Frequencies | 235.2241 | 236.9255 | 244.1004 |
| Frequencies | 247.189 | 253.2779 | 261.0747 |
| Frequencies | 262.8328 | 265.3567 | 270.5142 |
| Frequencies | 272.6223 | 277.088 | 287.0158 |
| Frequencies | 293.92 | 320.309 | 325.8315 |
| Frequencies | 335.6729 | 347.4429 | 353.8939 |
| Frequencies | 381.6219 | 391.2368 | 406.2437 |
| Frequencies | 423.0587 | 431.7228 | 438.817 |
| Frequencies | 457.5311 | 459.9967 | 467.7963 |
| Frequencies | 480.7396 | 486.8638 | 502.3434 |
| Frequencies | 504.0591 | 519.0013 | 535.7524 |
| Frequencies | 540.1959 | 566.6321 | 576.4803 |
| Frequencies | 587.3779 | 617.3986 | 631.7654 |
| Frequencies | 746.3521 | 757.3054 | 773.4244 |
| Frequencies | 778.6026 | 884.5584 | 896.1823 |
| Frequencies | 904.4903 | 962.0732 | 975.7488 |
| Frequencies | 989.2813 | 1585.374 | 1598.119 |
| Frequencies | 1633.634 | 1635.799 | 1636.031 |
| Frequencies | 1636.777 | 3630.629 | 3728.397 |
| Frequencies | 3754.187 | 3754.525 | 3782.863 |
| Frequencies | 3795.467 | 3806.22 | 3806.375 |
| Frequencies | 3808.291 | 3820.228 | 3849.317 |
| Frequencies | 3864.813 | 3869.829 | 3879.695 |
| Frequencies | 3884.586 | 3889.691 | 3898.866 |

**[(UO2)3(OH)7(H2O)]-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 22.5782 | 27.2733 | 44.7457 |
| Frequencies | 56.7839 | 62.261 | 74.0858 |
| Frequencies | 78.1529 | 84.3621 | 90.6909 |
| Frequencies | 97.5345 | 106.1847 | 120.5133 |
| Frequencies | 131.0283 | 134.2256 | 163.0589 |
| Frequencies | 169.3743 | 178.1246 | 190.2732 |
| Frequencies | 201.956 | 208.0422 | 214.4026 |
| Frequencies | 232.7025 | 243.5064 | 245.8172 |
| Frequencies | 252.8484 | 257.5648 | 259.333 |
| Frequencies | 265.7743 | 269.2235 | 279.5127 |
| Frequencies | 291.7803 | 302.2286 | 315.9115 |
| Frequencies | 339.4295 | 352.0778 | 353.0438 |
| Frequencies | 366.6816 | 374.0402 | 393.9541 |
| Frequencies | 408.7553 | 435.5743 | 444.2384 |
| Frequencies | 451.7593 | 465.7385 | 469.0088 |
| Frequencies | 476.7919 | 482.2357 | 511.5365 |
| Frequencies | 531.14 | 540.9404 | 546.5763 |
| Frequencies | 549.0581 | 713.6526 | 715.2257 |
| Frequencies | 716.6493 | 757.3835 | 823.3282 |
| Frequencies | 851.3684 | 858.7301 | 875.9324 |
| Frequencies | 910.429 | 913.8329 | 1585.002 |
| Frequencies | 3768.838 | 3811.277 | 3814.349 |
| Frequencies | 3818.33 | 3820.06 | 3837.383 |
| Frequencies | 3837.559 | 3838.396 | 3876.857 |

**[UO2SO4(H2O)4]**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 47.0668 | 56.6 | 62.084 |
| Frequencies | 76.3802 | 83.1746 | 94.1498 |
| Frequencies | 125.426 | 141.4247 | 142.9263 |
| Frequencies | 185.4988 | 193.8038 | 203.344 |
| Frequencies | 225.6292 | 233.5733 | 238.8029 |
| Frequencies | 255.4921 | 258.14 | 279.3889 |
| Frequencies | 294.7798 | 317.8567 | 323.5019 |
| Frequencies | 366.3681 | 426.3363 | 446.3653 |
| Frequencies | 452.8549 | 480.5269 | 494.6482 |
| Frequencies | 510.232 | 543.8411 | 561.6821 |
| Frequencies | 578.4023 | 610.676 | 640.8224 |
| Frequencies | 643.5506 | 729.473 | 895.4871 |
| Frequencies | 949.9702 | 978.521 | 1053.394 |
| Frequencies | 1144.256 | 1173.222 | 1287.638 |
| Frequencies | 1628.213 | 1634.058 | 1664.714 |
| Frequencies | 1676.74 | 2578.524 | 2642.347 |
| Frequencies | 3693.053 | 3790.797 | 3821.646 |
| Frequencies | 3829.884 | 3874.427 | 3897.909 |

**[UO2SO4(H2O)3]**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 41.2394 | 50.1317 | 60.8735 |
| Frequencies | 84.9698 | 104.8146 | 126.7288 |
| Frequencies | 133.1097 | 197.286 | 218.5539 |
| Frequencies | 225.5059 | 228.5181 | 237.9536 |
| Frequencies | 244.8284 | 252.6701 | 259.173 |
| Frequencies | 273.7683 | 291.9304 | 297.6718 |
| Frequencies | 303.5874 | 370.3327 | 392.2637 |
| Frequencies | 464.3368 | 490.9769 | 496.6955 |
| Frequencies | 544.2754 | 558.1228 | 564.508 |
| Frequencies | 597.0544 | 629.4556 | 836.3418 |
| Frequencies | 853.1764 | 863.7045 | 919.7239 |
| Frequencies | 974.539 | 1112.653 | 1308.258 |
| Frequencies | 1611.271 | 1640.894 | 1677.69 |
| Frequencies | 3208.912 | 3753.425 | 3804.621 |
| Frequencies | 3836.985 | 3855.24 | 3919.684 |

**[UO2(SO4)2(H2O)3]2-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 19.756 | 27.682 | 36.5366 |
| Frequencies | 61.2376 | 74.6933 | 83.2884 |
| Frequencies | 109.0978 | 124.7235 | 132.7356 |
| Frequencies | 154.2306 | 163.34 | 175.7649 |
| Frequencies | 186.6598 | 207.9636 | 234.1229 |
| Frequencies | 246.6063 | 252.3609 | 259.3677 |
| Frequencies | 261.517 | 290.9369 | 298.9807 |
| Frequencies | 336.7276 | 386.0518 | 418.9798 |
| Frequencies | 437.8928 | 445.2404 | 450.8973 |
| Frequencies | 479.1626 | 484.6717 | 545.8898 |
| Frequencies | 559.7713 | 565.2155 | 570.1389 |
| Frequencies | 599.9509 | 605.9085 | 621.8803 |
| Frequencies | 633.6902 | 635.9177 | 793.8129 |
| Frequencies | 850.8403 | 892.0533 | 930.5615 |
| Frequencies | 940.59 | 965.5391 | 1075.594 |
| Frequencies | 1116.021 | 1124.351 | 1154.814 |
| Frequencies | 1218.049 | 1245.635 | 1271.788 |
| Frequencies | 1621.07 | 1667.7 | 1674.946 |
| Frequencies | 2170.32 | 2793.736 | 2960.926 |
| Frequencies | 3842.426 | 3843.785 | 3858.752 |

**[UO2(SO4)2(H2O)2]2-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 19.55 | 39.605 | 71.7076 |
| Frequencies | 86.9622 | 90.6008 | 124.5316 |
| Frequencies | 129.3248 | 136.7537 | 179.0831 |
| Frequencies | 187.3136 | 209.7126 | 210.5064 |
| Frequencies | 215.0155 | 226.3274 | 243.5041 |
| Frequencies | 257.4452 | 258.5448 | 287.4211 |
| Frequencies | 300.8075 | 376.4227 | 419.0248 |
| Frequencies | 438.5038 | 469.2303 | 476.2359 |
| Frequencies | 488.152 | 545.1402 | 563.7886 |
| Frequencies | 568.2394 | 569.6707 | 597.9751 |
| Frequencies | 603.1847 | 617.5625 | 627.375 |
| Frequencies | 837.8466 | 863.0909 | 869.9576 |
| Frequencies | 885.6493 | 936.4309 | 962.488 |
| Frequencies | 1072.674 | 1087.295 | 1091.311 |
| Frequencies | 1134.645 | 1217.379 | 1250.627 |
| Frequencies | 1670.635 | 1674.377 | 2918.212 |
| Frequencies | 2966.72 | 3841.652 | 3842.598 |

**[UO2(SO4)2(H2O)]2-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 37.805 | 42.1958 | 68.4447 |
| Frequencies | 74.348 | 90.9487 | 128.0212 |
| Frequencies | 149.3703 | 155.3266 | 188.5179 |
| Frequencies | 207.4485 | 220.3569 | 226.1931 |
| Frequencies | 239.1252 | 242.3483 | 268.9194 |
| Frequencies | 303.0113 | 366.412 | 375.2158 |
| Frequencies | 386.2907 | 471.9392 | 486.4761 |
| Frequencies | 543.7862 | 546.7502 | 569.3506 |
| Frequencies | 571.1941 | 577.3472 | 596.9534 |
| Frequencies | 616.6302 | 829.6373 | 846.3275 |
| Frequencies | 865.4642 | 878.4795 | 882.0798 |
| Frequencies | 908.2063 | 936.7862 | 1126.527 |
| Frequencies | 1143.682 | 1249.478 | 1252.398 |
| Frequencies | 1649.243 | 3458.005 | 3835.681 |

**[UO2SO4(H2O)4(Ar-CH2N(CH3)3)]+**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 12.6025 | 16.0003 | 25.3996 |
| Frequencies | 36.1092 | 42.7971 | 46.9232 |
| Frequencies | 54.1474 | 60.2657 | 66.6215 |
| Frequencies | 71.1495 | 77.9423 | 80.5461 |
| Frequencies | 104.0180 | 112.4019 | 115.9013 |
| Frequencies | 120.8689 | 128.8979 | 147.4757 |
| Frequencies | 167.7008 | 188.2466 | 227.0960 |
| Frequencies | 234.3420 | 243.8596 | 248.5331 |
| Frequencies | 254.0844 | 257.3990 | 268.0355 |
| Frequencies | 275.0194 | 279.3264 | 288.1984 |
| Frequencies | 292.0389 | 296.7439 | 300.5533 |
| Frequencies | 325.0763 | 336.1732 | 366.2309 |
| Frequencies | 395.3157 | 417.4436 | 419.3331 |
| Frequencies | 444.2534 | 450.4253 | 450.9747 |
| Frequencies | 463.6570 | 484.1267 | 504.7211 |
| Frequencies | 525.8709 | 528.6711 | 544.7336 |
| Frequencies | 570.6917 | 574.6216 | 615.3077 |
| Frequencies | 621.4593 | 633.9923 | 711.7362 |
| Frequencies | 728.8610 | 788.1464 | 846.0772 |
| Frequencies | 863.7111 | 865.2671 | 873.0709 |
| Frequencies | 884.9304 | 901.4795 | 919.0000 |
| Frequencies | 946.0907 | 976.6886 | 980.6185 |
| Frequencies | 985.9524 | 993.8848 | 1017.0391 |
| Frequencies | 1019.1189 | 1056.5138 | 1087.8837 |
| Frequencies | 1114.6800 | 1141.8062 | 1144.3529 |
| Frequencies | 1155.3866 | 1194.2812 | 1213.1373 |
| Frequencies | 1226.1078 | 1237.3036 | 1257.8762 |
| Frequencies | 1267.7808 | 1293.9436 | 1334.3149 |
| Frequencies | 1365.3678 | 1376.0909 | 1401.8228 |
| Frequencies | 1458.3184 | 1464.3364 | 1489.0046 |
| Frequencies | 1494.5450 | 1497.2636 | 1501.3454 |
| Frequencies | 1507.6865 | 1512.7177 | 1536.6737 |
| Frequencies | 1538.3064 | 1540.4350 | 1542.5345 |
| Frequencies | 1626.7964 | 1638.9219 | 1640.0624 |
| Frequencies | 1641.2367 | 1658.3319 | 3070.0155 |
| Frequencies | 3075.2526 | 3082.1049 | 3089.6347 |
| Frequencies | 3145.4854 | 3166.3862 | 3174.2719 |
| Frequencies | 3178.7436 | 3183.1251 | 3184.9901 |
| Frequencies | 3185.9860 | 3194.0816 | 3199.5406 |
| Frequencies | 3202.5771 | 3212.4718 | 3221.6557 |
| Frequencies | 3723.5253 | 3775.8960 | 3801.9841 |
| Frequencies | 3862.5330 | 3872.2195 | 3907.2515 |

**[UO2(SO4)2(H2O)(Ar-CH2N(CH3)3)]-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 24.1023 | 31.7820 | 36.8236 |
| Frequencies | 44.4672 | 49.7460 | 56.0467 |
| Frequencies | 64.9035 | 75.8237 | 81.6634 |
| Frequencies | 87.6980 | 98.1437 | 106.0134 |
| Frequencies | 116.2515 | 131.2402 | 144.5543 |
| Frequencies | 151.4056 | 174.5554 | 193.5474 |
| Frequencies | 197.5554 | 212.1069 | 220.8446 |
| Frequencies | 226.6918 | 250.0310 | 253.5469 |
| Frequencies | 269.5910 | 271.5121 | 287.1480 |
| Frequencies | 294.5494 | 304.0043 | 307.4330 |
| Frequencies | 323.0969 | 339.9762 | 381.0503 |
| Frequencies | 384.3865 | 400.0256 | 423.2581 |
| Frequencies | 427.6700 | 458.1549 | 466.6097 |
| Frequencies | 470.1592 | 479.8108 | 526.5320 |
| Frequencies | 545.4858 | 548.1926 | 549.3340 |
| Frequencies | 570.6596 | 574.2043 | 598.1742 |
| Frequencies | 616.4439 | 622.8635 | 634.7974 |
| Frequencies | 715.9395 | 733.4899 | 782.9337 |
| Frequencies | 790.1693 | 846.3882 | 857.4676 |
| Frequencies | 870.1563 | 875.7613 | 884.0425 |
| Frequencies | 887.6629 | 889.5442 | 900.0491 |
| Frequencies | 931.4953 | 945.5663 | 947.9808 |
| Frequencies | 979.0605 | 989.2974 | 1011.3199 |
| Frequencies | 1014.8842 | 1041.0149 | 1058.2886 |
| Frequencies | 1090.5670 | 1105.9562 | 1115.0087 |
| Frequencies | 1129.6730 | 1145.1610 | 1156.8245 |
| Frequencies | 1186.8787 | 1217.6407 | 1234.2329 |
| Frequencies | 1240.9677 | 1254.3149 | 1263.7026 |
| Frequencies | 1269.6086 | 1295.8454 | 1335.3241 |
| Frequencies | 1369.6715 | 1379.9719 | 1418.0810 |
| Frequencies | 1452.2399 | 1465.3891 | 1478.2020 |
| Frequencies | 1490.6294 | 1501.2689 | 1502.7979 |
| Frequencies | 1506.5870 | 1517.0555 | 1521.6811 |
| Frequencies | 1530.9278 | 1542.5237 | 1544.3259 |
| Frequencies | 1637.5410 | 1655.4707 | 1661.4935 |
| Frequencies | 3062.0065 | 3071.3706 | 3078.4604 |
| Frequencies | 3083.3922 | 3138.9694 | 3166.8530 |
| Frequencies | 3167.3878 | 3169.5214 | 3176.1913 |
| Frequencies | 3177.7353 | 3181.7400 | 3188.3904 |
| Frequencies | 3195.1524 | 3199.1102 | 3205.1560 |
| Frequencies | 3233.5380 | 3518.3156 | 3843.4722 |

**[UO2(OH)SO4(H2O)2(Ar-CH2N(CH3)3)]**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 13.5600 | 17.0197 | 24.4961 |
| Frequencies | 40.2649 | 50.2269 | 52.0806 |
| Frequencies | 65.7496 | 68.9603 | 74.9952 |
| Frequencies | 84.6796 | 92.0101 | 119.1771 |
| Frequencies | 132.6570 | 133.7306 | 145.2131 |
| Frequencies | 152.3072 | 169.2537 | 196.3912 |
| Frequencies | 213.1383 | 226.7544 | 239.3705 |
| Frequencies | 252.4772 | 260.6494 | 267.6386 |
| Frequencies | 280.8550 | 282.2620 | 284.2049 |
| Frequencies | 290.9005 | 300.7436 | 313.8615 |
| Frequencies | 342.6468 | 356.6498 | 376.1750 |
| Frequencies | 400.5830 | 419.1812 | 420.5771 |
| Frequencies | 451.4252 | 466.0280 | 475.1200 |
| Frequencies | 477.3383 | 513.0644 | 515.3867 |
| Frequencies | 524.1656 | 530.3189 | 537.8896 |
| Frequencies | 557.4592 | 577.8941 | 606.0391 |
| Frequencies | 623.2336 | 634.6968 | 695.1002 |
| Frequencies | 713.7279 | 724.2622 | 730.9513 |
| Frequencies | 788.6094 | 846.4648 | 865.9882 |
| Frequencies | 870.3972 | 903.2449 | 916.6564 |
| Frequencies | 921.7470 | 944.2905 | 951.0962 |
| Frequencies | 966.3770 | 979.5426 | 983.8658 |
| Frequencies | 995.2049 | 1013.5669 | 1017.6071 |
| Frequencies | 1057.3349 | 1092.6069 | 1114.8378 |
| Frequencies | 1117.5052 | 1147.0322 | 1161.3109 |
| Frequencies | 1192.1456 | 1192.9973 | 1213.0529 |
| Frequencies | 1228.0944 | 1237.5345 | 1272.5329 |
| Frequencies | 1293.2561 | 1335.2230 | 1364.8651 |
| Frequencies | 1377.7364 | 1404.7569 | 1456.8198 |
| Frequencies | 1469.8249 | 1488.1562 | 1495.5017 |
| Frequencies | 1498.3884 | 1501.1726 | 1515.6953 |
| Frequencies | 1517.6370 | 1540.4668 | 1543.2234 |
| Frequencies | 1548.0975 | 1550.3414 | 1622.3537 |
| Frequencies | 1636.1822 | 1640.8617 | 1660.7815 |
| Frequencies | 3011.8782 | 3042.3193 | 3054.6020 |
| Frequencies | 3084.9276 | 3134.8319 | 3140.7384 |
| Frequencies | 3146.3214 | 3155.6088 | 3172.5403 |
| Frequencies | 3184.7607 | 3185.7260 | 3186.8193 |
| Frequencies | 3191.2255 | 3198.6463 | 3208.9326 |
| Frequencies | 3218.1250 | 3631.9949 | 3648.8286 |
| Frequencies | 3852.2289 | 3860.2454 | 3863.2124 |

**[(UO2)2(OH)(SO4)2(H2O)4(Ar-CH2N(CH3)3)]**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 8.3774 | 9.1619 | 15.5122 |
| Frequencies | 17.8317 | 27.5244 | 29.4203 |
| Frequencies | 31.1600 | 39.5517 | 43.3925 |
| Frequencies | 50.4944 | 51.3938 | 57.1177 |
| Frequencies | 63.4373 | 69.8361 | 79.1104 |
| Frequencies | 81.3590 | 89.1716 | 101.6992 |
| Frequencies | 105.8240 | 118.5009 | 123.0904 |
| Frequencies | 127.1070 | 131.7621 | 137.3122 |
| Frequencies | 140.2543 | 151.8946 | 167.3826 |
| Frequencies | 175.5274 | 185.4352 | 194.0140 |
| Frequencies | 203.0814 | 205.3128 | 214.7727 |
| Frequencies | 219.3873 | 227.7271 | 242.6814 |
| Frequencies | 256.4500 | 258.2664 | 268.6683 |
| Frequencies | 269.7420 | 270.5851 | 278.4478 |
| Frequencies | 286.6026 | 290.8955 | 299.5844 |
| Frequencies | 313.6877 | 322.6694 | 339.3002 |
| Frequencies | 348.4249 | 370.5361 | 378.9900 |
| Frequencies | 388.0660 | 393.4458 | 400.1454 |
| Frequencies | 401.2531 | 420.2417 | 423.6703 |
| Frequencies | 448.0687 | 449.6154 | 463.3275 |
| Frequencies | 482.3385 | 490.4269 | 493.5508 |
| Frequencies | 512.2952 | 524.2096 | 527.9161 |
| Frequencies | 534.2413 | 536.7518 | 551.7109 |
| Frequencies | 570.4667 | 576.1327 | 588.1384 |
| Frequencies | 596.0581 | 607.8760 | 616.3642 |
| Frequencies | 623.3318 | 634.9894 | 636.7368 |
| Frequencies | 696.5475 | 713.1410 | 730.3940 |
| Frequencies | 788.8319 | 795.3899 | 804.2949 |
| Frequencies | 808.7808 | 814.5704 | 847.4560 |
| Frequencies | 866.1699 | 871.8702 | 881.9196 |
| Frequencies | 895.9787 | 904.9028 | 913.3193 |
| Frequencies | 918.1096 | 921.7527 | 945.3289 |
| Frequencies | 962.2378 | 973.4204 | 978.4002 |
| Frequencies | 984.9856 | 998.7162 | 1015.9146 |
| Frequencies | 1017.5752 | 1057.2103 | 1093.2064 |
| Frequencies | 1116.2832 | 1129.3165 | 1152.2920 |
| Frequencies | 1153.7000 | 1155.1888 | 1193.1646 |
| Frequencies | 1212.9193 | 1218.1138 | 1229.3499 |
| Frequencies | 1237.6388 | 1273.9576 | 1289.3007 |
| Frequencies | 1293.2489 | 1335.9533 | 1365.2385 |
| Frequencies | 1378.8704 | 1381.0092 | 1404.9914 |
| Frequencies | 1459.3720 | 1468.2725 | 1490.5445 |
| Frequencies | 1493.7555 | 1498.5455 | 1504.0086 |
| Frequencies | 1513.8384 | 1515.5284 | 1537.9607 |
| Frequencies | 1540.7413 | 1543.8258 | 1548.8095 |
| Frequencies | 1600.2907 | 1628.5323 | 1637.2635 |
| Frequencies | 1640.7647 | 1660.3927 | 3036.4409 |
| Frequencies | 3062.1389 | 3071.2870 | 3089.1123 |
| Frequencies | 3144.3047 | 3144.9952 | 3162.1730 |
| Frequencies | 3171.1719 | 3172.4861 | 3184.4867 |
| Frequencies | 3185.5312 | 3189.7813 | 3192.4193 |
| Frequencies | 3199.6508 | 3209.7227 | 3219.0857 |
| Frequencies | 3380.3803 | 3574.0183 | 3610.9056 |
| Frequencies | 3695.9984 | 3793.4387 | 3797.8899 |
| Frequencies | 3824.3378 | 3837.0640 | 3867.4354 |

**[(UO2)2(OH)2(SO4)2(H2O)2(Ar-CH2N(CH3)3)]-**

|  |  |  |  |
| --- | --- | --- | --- |
| Frequencies | 16.7097 | 24.6481 | 29.6261 |
| Frequencies | 31.8912 | 37.4935 | 42.9706 |
| Frequencies | 52.2451 | 54.5986 | 58.2725 |
| Frequencies | 63.2823 | 72.4081 | 74.8858 |
| Frequencies | 81.7700 | 83.5382 | 89.4085 |
| Frequencies | 100.0304 | 102.5734 | 112.4117 |
| Frequencies | 116.4426 | 125.4190 | 127.3079 |
| Frequencies | 136.8666 | 155.9622 | 161.0470 |
| Frequencies | 180.7463 | 189.8920 | 205.0865 |
| Frequencies | 213.1543 | 216.1975 | 227.2237 |
| Frequencies | 236.3982 | 245.7368 | 257.8104 |
| Frequencies | 261.3599 | 270.9642 | 272.7817 |
| Frequencies | 278.3047 | 281.7261 | 297.4560 |
| Frequencies | 300.5127 | 308.2327 | 323.5013 |
| Frequencies | 339.7290 | 345.0610 | 352.2581 |
| Frequencies | 364.6257 | 378.0184 | 396.7650 |
| Frequencies | 400.2026 | 404.9932 | 421.6938 |
| Frequencies | 427.6828 | 430.5889 | 432.2581 |
| Frequencies | 452.8516 | 461.9774 | 468.1773 |
| Frequencies | 471.8219 | 489.8725 | 508.6777 |
| Frequencies | 530.5887 | 542.2240 | 552.2649 |
| Frequencies | 559.1799 | 570.5208 | 603.9592 |
| Frequencies | 611.9704 | 616.8297 | 623.2076 |
| Frequencies | 634.5934 | 645.7960 | 703.3881 |
| Frequencies | 714.4549 | 731.2336 | 768.4178 |
| Frequencies | 789.3392 | 803.2446 | 844.5043 |
| Frequencies | 846.4311 | 851.8882 | 869.8678 |
| Frequencies | 871.5797 | 874.8336 | 892.2785 |
| Frequencies | 896.6796 | 929.7534 | 941.5636 |
| Frequencies | 943.7051 | 955.2646 | 962.5091 |
| Frequencies | 981.8336 | 986.1728 | 1008.8218 |
| Frequencies | 1015.2994 | 1017.1071 | 1057.1483 |
| Frequencies | 1095.9807 | 1105.2085 | 1113.9865 |
| Frequencies | 1132.3953 | 1152.8180 | 1162.6577 |
| Frequencies | 1172.9740 | 1187.1036 | 1213.7261 |
| Frequencies | 1232.4068 | 1238.6621 | 1254.5385 |
| Frequencies | 1273.4763 | 1277.3950 | 1301.9521 |
| Frequencies | 1334.5982 | 1366.0753 | 1379.0614 |
| Frequencies | 1414.9017 | 1456.7355 | 1459.8129 |
| Frequencies | 1494.6369 | 1497.8050 | 1501.5095 |
| Frequencies | 1510.9032 | 1513.5856 | 1521.5225 |
| Frequencies | 1536.3142 | 1541.0069 | 1544.4103 |
| Frequencies | 1551.5241 | 1639.4074 | 1658.4623 |
| Frequencies | 1661.7022 | 1689.0656 | 2341.2503 |
| Frequencies | 3064.7716 | 3067.8832 | 3075.7207 |
| Frequencies | 3092.5304 | 3132.8394 | 3160.0446 |
| Frequencies | 3169.0798 | 3170.9569 | 3182.0307 |
| Frequencies | 3183.0472 | 3191.8577 | 3196.2100 |
| Frequencies | 3199.5132 | 3205.0272 | 3208.9002 |
| Frequencies | 3216.2915 | 3300.4709 | 3810.7746 |
| Frequencies | 3841.1710 | 3847.0967 | 3857.6526 |