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|--|--------------|--------------|--------------|
| Figure 1: HO-V⁴⁺OV⁴⁺-OH | | | |
| Coordinates (Angstroms) | | | |
| Atom | X | Y | Z |
| ----- | | | |
| Ti | 17.025616854 | 3.749890993 | 7.440788016 |
| Ti | 20.814816854 | 3.749890993 | 7.440788016 |
| Ti | 17.025616854 | -0.034309007 | 7.440788016 |
| Ti | 20.814816854 | -0.034309007 | 7.440788016 |
| O | 17.025616854 | 1.860290993 | 7.039188016 |
| O | 20.814816854 | 1.860290993 | 7.039188016 |
| O | 17.025616854 | 5.644490993 | 7.039188016 |
| O | 20.814816854 | 5.644490993 | 7.039188016 |
| O | 18.920216854 | -0.034309007 | 7.842288016 |
| O | 22.689416854 | -0.034309007 | 7.842288016 |
| O | 22.689416854 | 3.749890993 | 7.842288016 |
| O | 18.920216854 | 3.749890993 | 7.842288016 |
| Ti | 16.835991886 | 1.857242192 | 5.078060113 |
| Ti | 20.976578553 | 1.854306697 | 5.083330251 |
| Ti | 16.862547153 | 5.653913243 | 5.086364109 |
| Ti | 21.006468999 | 5.649148848 | 5.096933938 |
| O | 17.180421091 | 3.752577784 | 5.464442497 |
| O | 20.661573605 | 3.753616325 | 5.462978037 |
| O | 17.145384394 | -0.032393105 | 5.490610243 |
| O | 20.692692600 | -0.039732144 | 5.483535522 |
| O | 22.696572078 | 1.874142982 | 4.652552551 |
| O | 22.725896193 | 5.630942629 | 4.659751293 |
| O | 17.597294882 | 5.744874387 | 3.350944593 |
| O | 20.307909105 | 5.691869194 | 3.347120425 |
| O | 17.544439831 | 1.805758182 | 3.347044756 |
| O | 20.234333519 | 1.797597695 | 3.358954004 |
| V1 | 18.896120346 | 2.091968674 | 2.301623146 |
| V2 | 18.950346033 | 5.452455564 | 2.321345487 |
| O | 18.890069030 | 1.227136096 | 0.797392619 |
| O | 18.895729782 | 3.785021103 | 1.805846170 |
| O | 19.036969662 | 6.318626358 | 0.690042290 |
| H | 18.958146840 | 7.794594803 | 0.644610264 |
| H | 19.018234050 | 5.795202717 | -0.132873665 |

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| Figure 2: HO-V⁵⁺OV⁵⁺-OH | | | |
| Coordinates (Angstroms) | | | |
| Atom | X | Y | Z |
| ----- | | | |
| Ti | 17.025117458 | 3.714574372 | 7.442147147 |
| Ti | 20.814317458 | 3.714574372 | 7.442147147 |
| Ti | 17.025117458 | -0.069625628 | 7.442147147 |
| Ti | 20.814317458 | -0.069625628 | 7.442147147 |
| O | 17.025117458 | 1.824974372 | 7.040547147 |
| O | 20.814317458 | 1.824974372 | 7.040547147 |
| O | 17.025117458 | 5.609174372 | 7.040547147 |
| O | 20.814317458 | 5.609174372 | 7.040547147 |
| O | 18.919717458 | -0.069625628 | 7.843647147 |
| O | 22.688917458 | -0.069625628 | 7.843647147 |
| O | 22.688917458 | 3.714574372 | 7.843647147 |
| O | 18.919717458 | 3.714574372 | 7.843647147 |
| Ti | 16.846860072 | 1.817731807 | 5.044067580 |
| Ti | 20.973235739 | 1.816247743 | 5.050447017 |
| Ti | 16.837073621 | 5.607025461 | 5.063277054 |
| Ti | 20.975810385 | 5.605417797 | 5.068935326 |
| O | 17.112271873 | 3.716435016 | 5.503340028 |
| O | 20.710366678 | 3.714868116 | 5.499887247 |
| O | 17.174943161 | -0.071821371 | 5.484619018 |
| O | 20.644002161 | -0.071240471 | 5.477841816 |
| O | 22.701153931 | 1.754730447 | 4.670033156 |
| O | 22.698021147 | 5.657395890 | 4.673968139 |
| O | 17.504182576 | 5.545563465 | 3.372957231 |
| O | 20.295037358 | 5.537913150 | 3.381559889 |
| O | 17.526791257 | 1.961979639 | 3.365500370 |
| O | 20.305154340 | 1.972623518 | 3.361250159 |
| V1 | 18.918595618 | 2.162362062 | 2.270495476 |
| V2 | 18.905436687 | 5.934157776 | 2.362906298 |
| O | 18.904687477 | 3.771568493 | 1.957692855 |
| O | 18.909897524 | -0.022609009 | 2.467392888 |
| O | 18.945719578 | 1.625684431 | 0.548593683 |
| O | 18.916291630 | 5.931657818 | 0.538275838 |
| H | 18.951571596 | 8.229258984 | 0.424122151 |
| H | 18.910061564 | 5.018918898 | 0.178584757 |

Figure 3: $\text{H}_2\text{O}-\text{V}^{5+}\text{OV}^{5+}=\text{O}$
Coordinates (Angstroms)

| Atom | X | Y | Z |
|------|--------------|--------------|-------------|
| Ti | 17.311768626 | 3.642536591 | 7.382377893 |
| Ti | 21.100151476 | 3.685790679 | 7.316642755 |
| Ti | 17.354737480 | -0.141395334 | 7.368868281 |
| Ti | 21.143120330 | -0.098141246 | 7.303133143 |
| O | 17.326241827 | 1.754424748 | 6.974095007 |
| O | 21.114624676 | 1.797678836 | 6.908359870 |
| O | 17.283272973 | 5.538356672 | 6.987604620 |
| O | 21.071655823 | 5.581610760 | 6.921869482 |
| O | 19.255910005 | -0.121122249 | 7.737437732 |
| O | 23.024297168 | -0.078096463 | 7.672049554 |
| O | 22.981328314 | 3.705835462 | 7.685559167 |
| O | 19.212941152 | 3.662809676 | 7.750947344 |
| Ti | 17.242320761 | 1.736754779 | 4.942263875 |
| Ti | 21.372695976 | 1.811248063 | 4.934202057 |
| Ti | 17.110332805 | 5.528567291 | 5.029210704 |
| Ti | 21.254203345 | 5.594124412 | 4.941872921 |
| O | 17.449976978 | 3.652707053 | 5.430116096 |
| O | 21.016735077 | 3.706339505 | 5.373570750 |
| O | 17.473985045 | -0.183492812 | 5.429236981 |
| O | 21.029407840 | -0.090841316 | 5.350599437 |
| O | 23.090906954 | 1.773376797 | 4.466063412 |
| O | 22.980034832 | 5.568879154 | 4.558873544 |
| O | 17.809370444 | 5.403300040 | 3.319892683 |
| O | 20.505330075 | 5.654617541 | 3.241032759 |
| O | 18.098397628 | 1.597782823 | 3.407644589 |
| O | 20.574615577 | 1.976887387 | 3.338369525 |
| V | 19.387582313 | 1.953546791 | 1.999003570 |
| V | 19.136274314 | 5.269241964 | 2.203344032 |
| O | 20.277487375 | 1.156969081 | 0.925972820 |
| O | 19.260520835 | 3.646017658 | 1.479232068 |
| O | 18.884701837 | 6.332104569 | 1.001817639 |
| O | 17.745219509 | 1.142250821 | 0.902188308 |
| H | 18.069597456 | 0.202550828 | 0.732073888 |
| H | 16.965370047 | 1.064456432 | 1.490924383 |

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| Figure 5: INT | | | |
| Coordinates (Angstroms) | | | |
| Atom | X | Y | Z |
| ----- | | | |
| Ti | 17.087730611 | 3.877550366 | 7.312263218 |
| Ti | 20.876478482 | 3.852032976 | 7.261485542 |
| Ti | 17.062343055 | 0.093473877 | 7.319997611 |
| Ti | 20.851090925 | 0.067956487 | 7.269219935 |
| O | 17.069663954 | 1.987226270 | 6.914562979 |
| O | 20.858411824 | 1.961708880 | 6.863785304 |
| O | 17.095051511 | 5.771302759 | 6.906828587 |
| O | 20.883799381 | 5.745785369 | 6.856050911 |
| O | 18.962105298 | 0.081500757 | 7.696071108 |
| O | 22.730855554 | 0.056118051 | 7.645561444 |
| O | 22.756243112 | 3.840194541 | 7.637827053 |
| O | 18.987492856 | 3.865577246 | 7.688336715 |
| Ti | 16.871752992 | 1.961101524 | 4.892970540 |
| Ti | 21.003882362 | 1.971289949 | 4.831715573 |
| Ti | 16.935523028 | 5.759008175 | 4.965752527 |
| Ti | 21.092755203 | 5.767493711 | 4.921158588 |
| O | 17.183543557 | 3.874266542 | 5.363614585 |
| O | 20.752433901 | 3.896912547 | 5.300313984 |
| O | 17.149242159 | 0.061441405 | 5.378791915 |
| O | 20.743137409 | 0.051826435 | 5.318270167 |
| O | 22.735720931 | 1.983459628 | 4.370377340 |
| O | 22.808267362 | 5.747301884 | 4.491491689 |
| O | 17.776817776 | 5.656157615 | 3.295457821 |
| O | 20.449456914 | 5.937044146 | 3.139419281 |
| O | 17.723573033 | 1.842909365 | 3.367643608 |
| O | 20.134898298 | 2.051192425 | 3.310126513 |
| V1 | 18.865150193 | 2.224689238 | 1.898594443 |
| V2 | 19.098805656 | 5.527939214 | 2.176160291 |
| O | 19.673651577 | 1.239881322 | 0.860176036 |
| O | 19.337651628 | 3.936481898 | 1.559612992 |
| O | 18.900148418 | 6.525499702 | 0.817706823 |
| O | 17.302251496 | 2.249500380 | 0.970180743 |
| H | 19.271049659 | -0.046868998 | 0.732058858 |
| H | 16.478082812 | 2.415303816 | 1.471655487 |