***List of Filenames***

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | | Filename | cm-1 | cm-1 | ppm |
| **BVP Geometries** | |  |  |  |  |
| 6 BVP molecules | | BVP\_6 |  | 1682 | 172.6 |
| 6 BVP molecules, 12 H2O molecules, 2 AB-ribbons | | BVP\_6\_H2O\_12\_AB\_2 | 3441 | 1642 | 176.9 |
| 6 BVP molecules, 6 H2O molecules at B, 6 H2O2 molecules at A, 2 AB-ribbons | | BVP\_6\_H2O\_6B\_H2O2\_6A\_AB\_2 | 3405 | 1633 | 177.9 |
| 6 BVP molecules, 6 H2O molecules at A, 6 H2O2 molecules at B, 2 AB-ribbons | | BVP\_6\_H2O\_6A\_H2O2\_6B\_AB\_2 | 3253 | 1641 | 176.8 |
| 6 BVP molecules, 1 H2O molecule at B, 11 H2O2 molecules, 2 AB-ribbons | | BVP\_6\_H2O\_1B\_H2O2\_11\_AB\_2 | 3316 | 1638 |  |
| 6 BVP molecules, 1 H2O molecule at A, 11 H2O2 molecules, 2 AB-ribbons | | BVP\_6\_H2O\_1A\_H2O2\_11\_AB\_2 | 3305 | 1639 |  |
| 6 BVP molecules, 12 H2O2 molecules, 2 AB-ribbons | | BVP\_6\_H2O2\_12\_AB\_2 | 3311 | 1637 | 178.4 |
| 6 BVP molecules, 12 H2O2 molecules, 2 A-ribbons | | BVP\_6\_H2O2\_12\_A\_2 | 3191 | 1652 | 177.2 |
| 6 BVP molecules, 12 H2O2 molecules, 3 A-ribbons | | BVP\_6\_H2O2\_12\_A\_3 | 3243 | 1644 | 176.3 |
|  | |  |  |  |  |
| 6 BVP molecules, 12 H2O2 molecules, 2 AB-ribbons X-ray H-optimised | | BVP\_6\_XR\_Hopt | 3337 | 1661 | 173.8 |
|  | |  |  |  |  |
| 2 BVP molecules, 4 H2O2 molecules, 1 A-ribbon | | BVP\_2\_H2O2\_4 | 3316 | 1655 | 177.1 |
| 3 BVP molecules, 6 H2O2 molecules, 1 A-ribbon | | BVP\_3\_H2O2\_6 | 3234 | 1655 | 178.1 |
|  | |  |  |  |  |
| **PVP Tetramer Geometries** | |  |  |  |  |
| 3 PVP4 molecules | | PVP4\_3 |  | 1690 | 173.7 |
| 3 PVP4 molecules, 12 H2O molecules, 2 AB-ribbons | | PVP4\_3\_H2O\_12\_AB\_2 | 3471 | 1655 | 176.5 |
| 3 PVP4 molecules, 6 H2O molecules at B, 6 H2O2 molecules at A, 2 AB-ribbons | | PVP4\_3\_H2O\_6B\_H2O2\_6A\_AB\_2 | 3220 | 1650 | 175.4 |
| 3 PVP4 molecules, 6 H2O molecules at A, 6 H2O2 molecules at B, 2 AB-ribbons | | PVP4\_3\_H2O\_6A\_H2O2\_6B\_AB\_2 | 3132 | 1645 | 176.6 |
| 3 PVP4 molecules, 1 H2O molecule at B, 11 H2O2 molecules, 2 AB-ribbons | | PVP4\_3\_H2O\_1B\_H2O2\_11\_AB\_2 | 3312 | 1647 |  |
| 3 PVP4 molecules, 1 H2O molecule at A, 11 H2O2 molecules, 2 AB-ribbons | | PVP4\_3\_H2O\_1A\_H2O2\_11\_AB\_2 | 3297 | 1644 |  |
| 3 PVP4 molecules, 12 H2O2 molecules, 2 AB-ribbons | | PVP4\_3\_H2O2\_12\_AB\_2 | 3293 | 1643 | 177.8 |
| 3 PVP4 molecules, 12 H2O2 molecules, 2 A-ribbons | | PVP4\_3\_H2O2\_12\_A\_2 | 3149 | 1649 | 178.1 |
| 3 PVP4 molecules, 12 H2O2 molecules, 3 A-ribbons | | PVP4\_3\_H2O2\_12\_A\_3 | 3190 | 1647 | 177.7 |
|  | |  |  |  |  |
| **PVP Hexamer Geometries** | |  |  |  |  |
| 2 PVP6 molecules | | PVP6\_2 |  | 1688 | 174.4 |
| 2 PVP6 molecules, 12 H2O2 molecules, 2A-ribbons | | PVP6\_2\_H2O2\_12\_A\_2 | 3300 | 1652 | 179.0 |
|  | |  |  |  |  |
| 1 PVP6 molecule | | PVP6\_1 |  | 1698 | 174.1 |
| 1 PVP6 molecule, 6 H2O2 molecules, 1A-ribbon | | PVP6\_1\_H2O2\_6\_A | 3290 | 1654 | 178.9 |
|  |  | |  |  |  |