Supplementary Information

**A Combined Spectroscopic and Computational Investigation on the Oxidation of *exo*-Tetrahydrodicyclopentadiene (JP-10; C10H16) Doped with Titanium-Aluminum-Boron Reactive Metal Nanopowder**

**SUPPLEMENTARY INFORMATION**

Stephen J. Brotton, Sahan D. Perera, Anupam Misra, N. Fabian Kleimeier, Andrew M. Turner, Ralf I. Kaiser\*

*Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, USA*

Mark Palenik, Matthew T. Finn, Albert Epshteyn\*

*U.S. Naval Research Laboratory, Washington, DC 20375, USA*

Bing-Jian Sun, Li-Jie Zhang, Agnes H. H. Chang\*

*Department of Chemistry, National Dong Hwa University, Shoufeng, Hualien 974, Taiwan*



Figure S1: Calibration curves used to calibrate the (a) low energy region of Raman data (100 cm−1 – 2400 cm−1) and (b) high energy region of Raman data (2200 cm−1 – 4000 cm−1). Each region was calibrated with cyclohexane (red), toluene (blue) and acetonitrile (green) respectively. The graphs were fit with the following second order polynomials: (a) and (b) .



Figure S2: Comparison between the calculated vibrational wavenumber and (a) the experimental Raman wavenumber and (b) the experimental FTIR wavenumber of the normal modes of e*xo*-tetrahydrodicyclopentadiene. Both the lower energy (red; 100 – 1100 cm-1) and high energy region (blue; 1120 – 3100 cm-1) of each plot were linearly fit to obtain a scaling factor for each region of 0.99 and 0.94 for Raman and 0.98 and 0.94 for FTIR, respectively.



Figure S3: Overview Raman spectra of (a) JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 100 – 4,000 cm-1 region.



Figure S4: Raman spectra of (a) pure JP-10, (b) JP-10-Al, (c) JP-10-Ti-Al-B NPs (RMNPs), and (d) Ti-Al-BNPs (RMNPs) in the 100 – 350 cm-1 region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S5: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 350 – 600 cm-1 region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S6: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 600 – 1,100 cm-1 region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S7: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 1,100 – 1,800 cm-1 region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S8: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 2,500 – 4,000 cm-1 region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S9: FTIR spectra of pure JP-10 in the 500 – 4,000 cm-1 region



Figure S10: FTIR spectra of JP-10 in the (a) 500 –1,100 cm-1 (b) 1,100 – 1,800 cm-1, and (c) 2,000 –4,000 cm-1 region. The overall fit and individual peak fits in each region are shown in red and green, respectively. Peak assignments are compiled in Table S1.



Figure S11: Raman spectra of new peaks resulting from photochemically activated JP-10-Ti-Al-B NPs (RMNPs) by a tightly focused 532 nm laser beam (45 – 50 µm) at 1 kHz

Table S1: Vibrational Mode Assignments for the Observed Peaks in the Raman Spectra of JP-10, JP-10-Al, and JP-10-Ti-Al-B NPs (RMNPs), Ti-Al-B NPs (RMNPs), and the FTIR Spectra of JP-10.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Normal Mode | Raman Wavenumber (cm-1)  JP-10 | Raman Wavenumber (cm-1)  JP-10  Al | Raman Wavenumber (cm-1)  JP-10  Ti-Al-B NPs | Raman Wavenumber (cm-1)  Ti-Al-B NPs | FTIR Wavenumber (cm-1)  JP-10 | Calculated Wavenumber(cm-1)  JP-10 | Calculated FTIR Intensity  JP-10 | Vibrational Mode Assignment\* |
| ν1 | - | - | - | - | - | 140 | 0.009 | Ring twist |
| ν2 | 188 | 188 | 192 |  | - | 177 | 0.003 | CCC bend |
| νA | - | - | 227 | 231 | - | - | - | Al-B stretch |
| νB | - | - | 267 | 267 | - | - | - | Ti-B stretch |
| ν3 | 271 | 270 | 297 | - | - | 270 | 0.068 | CCC bend |
| ν4 | - | - | - | - | - | 317 | 0.028 | CH2 rock |
| ν5 | - | - | - | - | - | 319 | 0.046 | Ring twist |
| ν6 | 401 | 401 | 401 | - | - | 398 | 0.043 | CCC bend |
| ν7 | 490 | 490 | 482 | - | 513 | 495 | 0.237 | CCC bend |
| ν8 | 532 | 531 | 525 | - | 528 | 534 | 0.180 | Ring twist |
| ν9 | 551 | 551 | 544 | - | 554 | 554 | 0.661 | CCC bend |
| ν10 | - | - | 660\* | - | 659 | 671 | 0.678 | Ring rock |
| ν11 | 732 | 732 | 740 | - | 733 | 739 | 0.369 | Ring rock |
| ν12 | 744 | 743 | - | 745 | 753 | 0.356 | CC stretch |
| ν13 | 783 | 783 | 782 | - | 783 | 792 | 1.292 | CC stretch |
| ν14 | 814 | 813 | 813 | - | 816 | 828 | 0.643 | CH2 rock |
| ν15 | 853 | 852 | 845 | - | - | 864 | 0.067 | CCC bend |
| ν16 | - | 855 | 865 | 1.181 | CCC bend |
| ν17 | 879 | 879 | 879 | - | 883 | 889 | 0.626 | CCC rock |
| ν18 | 903 | 903 | 910 | - | - | 894 | 0.116 | CC stretch |
| ν19 | 914 | 914 | - | 907 | 913 | 0.882 | Ring stretch |
| ν20 | - | - | - | - | - | 918 | 0.041 | CH2bend/rock |
| ν21 | - | - | - | - | 918 | 926 | 1.102 | CCC rock |
| ν22 | 945 | 944 | 941 | - | 945 | 955 | 2.044 | Ring breathing |
| ν23 | - | - | - | - | - | 963 | 0.045 | CC stretch |
| ν24 | 980 | 980 | 976 | - | 980 | 992 | 1.882 | CC stretch |
| ν25 | - | - | - | - | 988 | 999 | 0.806 | CH2 bend |
| ν26 | 1030 | 1030 | 1040 | - | 1032 | 1041 | 0.206 | CH2 twist |
| ν27 | 1050 | 1049 | - | - | 1050 | 0.488 | CH2 bend |
| ν28 | - | 1057 | 1052 | 0.083 | CH2 rock |
| ν29 | - | - | 1054 | 0.001 | CH2 bend |
| ν30 | 1107 | 1106 | 1157 | - | 1113 | 1073 | 0.780 | CH2 twist/rock |
| ν31 | 1126 | 1124 | - | 1129 | 1138 | 0.097 | CH2 wag |
| ν32 | 1138 | 1138 | - | - | 1153 | 0.026 | CH2 twist |
| ν33 | 1161 | 1160 | - | 1144 | 1169 | 1.210 | CH2 twist |
| ν34 | 1196 | 1196 | - | 1179 | 1193 | 0.188 | CH2 wag |
| ν35 | - | - | - | - | 1204 | 0.068 | CH2 rock |
| ν36 | - | - | - | 1186 | 1209 | 1.777 | CH2 bend |
| ν37 | 1219 | 1219 | - | 1201 | 1227 | 1.564 | CH2 bend |
| ν38 | - | - | - | - | - | 1251 | 0.018 | CH2 twist |
| ν39 | - | - | - | - | 1233 | 1261 | 0.807 | CH2 twist |
| ν40 | 1276 | 1275 | 1315 | - | 1254 | 1289 | 1.3410 | CH2 wag |
| ν41 | - | - | - | - | 1301 | 0.0411 | CH wag |
| ν42 | 1304 | 1303 | - | 1270 | 1306 | 0.1915 | CH2 wag |
| ν43 | - | - | - | - | 1312 | 0.372 | CH2 wag |
| ν44 | - | - | - | - | 1317 | 0.002 | CH2 wag |
| ν45 | 1327 | 1328 | - | 1277 | 1327 | 0.051 | CH2 wag |
| ν46 | - | 1297 | 1331 | 1.908 | CH2 wag |
| ν47 | - | - | - | - | 1310 | 1343 | 0.680 | CH wag |
| ν48 | - | - | - | - | 1318 | 1349 | 0.982 | CH2 wag |
| ν49 | - | - | - | - | 1330 | 1367 | 1.003 | CH2 wag |
| ν50 | - | - | - | - | - | 1372 | 0.514 | CH2 twist |
| ν51 | 1420 | 1420 | 1431 | - | - | 1492 | 0.776 | CH wag |
| ν52 | - | - | 1494 | 2.166 | CH2 rock |
| ν53 | - | - | 1496 | 1.794 | CH2 rock |
| ν54 | 1444 | 1442 | - | 1456 | 1503 | 6.403 | CH2 scissor |
| ν55 | 1465 | 1463 | - | 1468 | 1514 | 11.009 | CH2 scissor |
| ν56 | - | - | - | - | 1475 | 1526 | 4.457 | CH2 rock |
| 2ν13 | - | - | 1560 | - | - | - | - | overtone |
| 2ν17 | - | - | 1728 | - | - | - | - | overtone |
| ν57 | 2870 | 2869 | 2866 | - | 2865 | 3016 | 20.073 | CH stretch |
| ν58 | - | - | 3021 | 30.463 | CH stretch |
| ν59 | - | - | 3024 | 22.102 | CH stretch |
| ν60 | - | - | 3030 | 1.097 | CH2 stretch |
| ν61 | - | - | 3034 | 25.961 | CH2 stretch |
| ν62 | 2910 | 2910 | 2915 | - | 2913 | 3042 | 58.93 | CH2 stretch |
| ν63 | - | - | 3044 | 12.198 | CH2 stretch |
| ν64 | - | - | 3046 | 66.233 | CH2 stretch |
| ν65 | 2954 | 2953 | 2951 | - | - | 3065 | 6.172 | CH2 stretch |
| ν66 | - | - | 3068 | 46.085 | CH stretch |
| ν67 | - | - | 3071 | 38.453 | CH stretch |
| ν68 | - | 2942 | 3073 | 104.144 | CH stretch |
| ν69 | - | - | 3077 | 49.579 | CH stretch |
| ν70 | - | - | 3080 | 9.511 | CH stretch |
| ν71 | - | - | - | - | - | 3087 | 85.784 | CH2 stretch |
| ν72 | - | - | - | - | - | 3088 | 61.510 | CH2 stretch |

Table S2: Total reaction energies (ΔE) and zero point energy corrected reaction energies (ΔE+ΔZPE) for the hydrogen abstraction channels of aluminum, boron, and titanium leading to the mono hydrides plus the corresponding JP-10 radical R1 to R6 refer (Figure 2). The Cartesian coordinates and vibrational modes are compiled in Table S6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| reactants | ΔE  B3LYP/def2-TZVP | ΔE +ΔZPE  B3LYP/ def2-TZVP | ΔE  MP2/6-311g\* | ΔE +ΔZPE  MP2/6-311g\* |
|  | products | |  |  |
| JP-10 + Al | R1 + AlH  129 | R1 + AlH  91 | R1 + AlH  159 | R1 + AlH  131 |
|  | R2 + AlH  162 | R2 + AlH  129 | R2 + AlH  192 | R2 + AlH  169 |
|  | R3 + AlH  151 | R3 + AlH  113 | R3 + AlH  180 | R3 + AlH  153 |
|  | R4 + AlH  131 | R4 + AlH  93 | R4 + AlH  164 | R4 + AlH  138 |
|  | R5 + AlH  124 | R5 + AlH  84 | R5 + AlH  156 | R5 + AlH  127 |
|  | R6 + AlH  126 | R6 + AlH  85 | R6 + AlH  159 | R6 + AlH  130 |
| JP-10 + B | R1 + BH  160 | R1 + BH  135 | R1 + BH  111 | R1 + BH  88 |
|  | R2 + BH  193 | R2 + BH  173 | R2 + BH  145 | R2 + BH  125 |
|  | R3 + BH  182 | R3 + BH  158 | R3 + BH  132 | R3 + BH  109 |
|  | R4 + BH  162 | R4 + BH  139 | R4 + BH  116 | R4 + BH  94 |
|  | R5 + BH  155 | R5 + BH  129 | R5 + BH  108 | R5 + BH  84 |
|  | R6 + BH  157 | R6 + BH  131 | R6 + BH  111 | R6 + BH  86 |
| JP-10 + Ti | R1 + TiH  253 | R1 + TiH  223 | R1 + TiH  272 | R1 + TiH  243 |
|  | R2 + TiH  287 | R2 + TiH  262 | R2 + TiH  305 | R2 + TiH  281 |
|  | R3 + TiH  274 | R3 + TiH  245 | R3 + TiH  293 | R3 + TiH  265 |
|  | R4 + TiH  255 | R4 + TiH  228 | R4 + TiH  277 | R4 + TiH  251 |
|  | R5 + TiH  247 | R5 + TiH  217 | R5 + TiH  269 | R5 + TiH  240 |
|  | R6 + TiH  250 | R6 + TiH  220 | R6 + TiH  272 | R6 + TiH  242 |

Table S3: Total energies (ΔE) and zero point energy corrected total energies (ΔE+ΔZPE) computed with MP2/6-311g\* for the initial van-der-Waals (vdW) complexes (vdW I), transition states (TS), final van-der-Waals (vdW II) complexes, and products during the reaction of aluminum monoxide (AlO) and boron monoxide (BO) with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S6.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| reactants | E | E+ZPE |  | E+ ZPE |  | E+ ZPE |  | E+ ZPE |
|  | vdW I | | TS | | vdW II | | products | |
| JP-10 + BO | -9 | -8 | 23 | 8 | -37 | -46 | -29 | R1 + HBO  -41 |
|  | -7 | -6 | 35 | 21 | -5 | -11 | 4 | R2 + HBO  -3 |
|  | -11 | -10 | 42 | 28 | -15 | -24 | -8 | R3 + HBO  -19 |
|  | -10 | -9 | 15 | 1 | -33 | -42 | -24 | R4 + HBO  -34 |
|  | -9 | -7 | 28 | 14 | -38 | -49 | -322 | R5 + HBO  -45 |
|  | -11 | -10 | 23 | 8 | -43 | -54 | -29 | R6 + HBO  -42 |
| JP-10 + AlO | 42 | 3 | 58 | 6 | -60 | -106 | -36 | R1 + AlOH  -90 |
|  | 42 | 3 | 55 | 8 | -28 | -71 | -3 | R2 + AlOH  -52 |
|  | -33 | -48 | 53 | 4 | -40 | -85 | -15 | R3 + AlOH  -68 |
|  | -33 | -8 | 45 | 8 | -59 | -104 | -39 | R4 + AlOH  -82 |
|  | -33 | -8 | 61 | 8 | -58 | -106 | -39 | R5 + AlOH  -93 |
|  | -33 | -8 | 65 | 20 | -61 | -109 | -39 | R6 + AlOH  -91 |

Table S4: Total energies (ΔE) and zero point energy corrected total energies (ΔE+ΔZPE) for the transition states, final van-der-Waals (vdW) complexes (vdW II), and products during the reaction of boron dioxide (BO2) with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S6.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| reactants | ΔE | ΔE+ ΔZPE | ΔE | ΔE+ ΔZPE | ΔE | ΔE+ ΔZPE |
|  | TS | | vdW II | | products | |
| JP-10 + BO2 | 10 | 17 | -97 | -85 | -62 | R1 + BO2H  -56 |
|  | 9 | 19 | -69 | -56 | -29 | R2 + BO2H  -35 |
|  | 14 | 13 | -73 | -62 | -41 | R3 + BO2H  -35 |
|  | 5 | 5 | -99 | -87 | -57 | R4 + BO2H  -49 |
|  | 15 | 23 | -100 | -89 | -65 | R5 + BO2H  -60 |
|  | 30 | 29 | -93 | -83 | -62 | R6 + BO2H  -58 |

Table S5: Total energies (ΔE) and zero point energy corrected total energies (ΔE+ΔZPE) for van-der-Waals (vdW) complexes in the exit channel (vdW II), transition state to insertion (TS), the intermediates, and products accessed during the reaction of atomic and molecular oxygen with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S7.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| reactants | ΔE | ΔE+ΔZPE | ΔE | ΔE+ΔZPE | | ΔE | ΔE +ΔZPE |
|  | TS | | vdW II complex | | | products | |
| JP-10 + O | 49 | 34 | -4 | | -13 | R1 + OH  14 | R1 + OH  -2 |
|  | 60 | 43 | 26 | | 20 | R2 + OH  46 | R2 + OH  34 |
|  | 59 | 43 | 18 | | 8 | R3 + OH  35 | R3 + OH  19 |
|  | 42 | 28 | -4 | | -12 | R4 + OH  18 | R4 + OH  3 |
|  | 49 | 33 | -6 | | -17 | R5 + OH  11 | R5 + OH  -6 |
|  | 50 | 34 | -4 | | -15 | R6 + OH  14 | R6 + OH  -4 |
| reactants | ΔE | ΔE+ ΔZPE | ΔE | | ΔE+  ΔZPE | ΔE | ΔE +ΔZPE |
|  | TS | | VdW complex | | | products | |
| JP-10 + O2 | 210 | 196 | 197 | | 191 | R1 + O2H  217 | R1 + O2H  206 |
|  | 230 | 224\* | 222 | | 227 | R2 + O2H  249 | R2 + O2H  242 |
|  | 218 | 209 | 215 | | 208 | R3 + O2H  237 | R3 + O2H  227 |
|  | 205 | 199 | 193 | | 197 | R4 + O2H  220 | R4 + O2H  211 |
|  | 205 | 190 | 190 | | 183 | R5 + O2H  213 | R5 + O2H  202 |
|  | 202 | 188 | 192 | | 184 | R6 + O2H  217 | R6 + O2H  204 |

\* This transition state could not be located at the B3LYP/cc-pVTZ level of theory. MP2/cc-pVDZ does locate the transition state; however, with zero-point energy correction (either with harmonic or anharmonic frequencies), the energy is found lower than the corresponding R2-OOH van-der-Waals complex and likewise for CCSD/cc-pVTZ energy.

Table S6: Cartesian coordinates and vibrational frequencies of van-der-Waals complexes, transition states and products of the reactions of BO, AlO, and BO2 with JP-10. Calculations are performed at the MP2/6-311g\* level unless otherwise indicated.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom | X | Y | Z |  |
| **JP-10** | | | |  |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.362754 | -0.785814 | -0.514719 | | C | -0.362754 | 0.785811 | -0.514726 | | C | 0.879767 | -1.131868 | 0.324589 | | C | 0.879774 | 1.131874 | 0.32457 | | C | 0.888333 | 0.000014 | 1.367226 | | C | 2.128868 | -0.779704 | -0.505758 | | C | 2.128874 | 0.779688 | -0.505769 | | C | -1.718206 | -1.199374 | 0.088531 | | C | -1.7182 | 1.199373 | 0.088531 | | C | -2.63457 | 0.000002 | -0.18068 | | H | -0.269974 | -1.189074 | -1.531257 | | H | -0.269983 | 1.189061 | -1.531269 | | H | 0.877652 | -2.154287 | 0.718985 | | H | 0.877666 | 2.154302 | 0.718943 | | H | 0.017186 | 0.000022 | 2.028639 | | H | 1.793214 | 0.000017 | 1.985804 | | H | 2.080761 | -1.204432 | -1.513657 | | H | 3.03321 | -1.171596 | -0.028391 | | H | 3.033218 | 1.171577 | -0.028402 | | H | 2.080776 | 1.204402 | -1.513674 | | H | -1.619754 | -1.353279 | 1.170221 | | H | -2.091151 | -2.135852 | -0.33893 | | H | -2.091143 | 2.135854 | -0.338926 | | H | -1.619744 | 1.353272 | 1.170222 | | H | -2.945458 | 0 | -1.232529 | | H | -3.541266 | 0.000002 | 0.433452 | | | | |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R1** | | | | **R2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.354 | 0.792227 | -0.528413 | | C | 0.302153 | -0.778172 | -0.515397 | | C | -0.89737 | 1.179636 | 0.306674 | | C | -0.948358 | -1.087524 | 0.331605 | | C | -0.919575 | 0.055 | 1.363006 | | C | -2.093616 | 0.799885 | -0.519299 | | C | -2.193808 | -0.70807 | -0.499451 | | C | 1.716735 | 1.171174 | 0.082399 | | C | 1.644532 | -1.229103 | 0.090346 | | C | 2.597116 | -0.057416 | -0.178149 | | H | 0.276556 | 1.189579 | -1.5475 | | H | 0.195433 | -1.184508 | -1.529229 | | H | -0.884381 | 2.209211 | 0.678687 | | H | -0.969804 | -2.104778 | 0.737439 | | H | -0.038942 | 0.04115 | 2.011143 | | H | -1.817305 | 0.086288 | 1.989169 | | H | -2.515721 | 1.42909 | -1.296802 | | H | -3.114517 | -1.050831 | -0.00374 | | H | -2.18461 | -1.160241 | -1.499772 | | H | 1.617999 | 1.334378 | 1.162481 | | H | 2.119161 | 2.093162 | -0.349509 | | H | 1.991754 | -2.17615 | -0.335407 | | H | 1.540128 | -1.379575 | 1.171964 | | H | 2.91244 | -0.069828 | -1.228573 | | H | 3.500956 | -0.082762 | 0.439729 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.368548 | -0.850808 | -0.463545 | | C | -0.33928 | 0.734012 | -0.552709 | | C | 0.8699 | -1.101186 | 0.369201 | | C | 0.908734 | 1.108559 | 0.276113 | | C | 0.88935 | 0.028682 | 1.387578 | | C | 2.136753 | -0.880453 | -0.434369 | | C | 2.166287 | 0.689611 | -0.518723 | | C | -1.72899 | -1.198294 | 0.167924 | | C | -1.690504 | 1.19882 | 0.019876 | | C | -2.623542 | -0.001658 | -0.17772 | | H | -0.282434 | -1.307976 | -1.456254 | | H | -0.23396 | 1.07083 | -1.591798 | | H | 0.918882 | 2.152385 | 0.610805 | | H | 0.010929 | 0.075407 | 2.034986 | | H | 1.791889 | 0.041717 | 2.00679 | | H | 2.097222 | -1.35714 | -1.41764 | | H | 3.018605 | -1.260235 | 0.090984 | | H | 3.071978 | 1.088375 | -0.050091 | | H | 2.139277 | 1.053781 | -1.550665 | | H | -1.629882 | -1.289217 | 1.255495 | | H | -2.117367 | -2.15221 | -0.201788 | | H | -2.049267 | 2.111606 | -0.467007 | | H | -1.59262 | 1.41917 | 1.089928 | | H | -2.933159 | -0.061076 | -1.228294 | | H | -3.531043 | 0.050878 | 0.432792 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R3** | | | | **R4** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.356909 | -0.786935 | -0.498841 | | C | -0.356909 | 0.786936 | -0.498842 | | C | 0.876342 | -1.136847 | 0.35768 | | C | 0.876343 | 1.136848 | 0.357677 | | C | 0.876694 | 0.000002 | 1.352077 | | C | 2.13995 | -0.780727 | -0.469251 | | C | 2.139951 | 0.780725 | -0.469253 | | C | -1.709529 | -1.195627 | 0.111241 | | C | -1.709529 | 1.195626 | 0.111242 | | C | -2.627118 | 0 | -0.165467 | | H | -0.258293 | -1.19347 | -1.513472 | | H | -0.258294 | 1.19347 | -1.513473 | | H | 0.872829 | -2.154934 | 0.75836 | | H | 0.872831 | 2.154936 | 0.758356 | | H | 1.434973 | 0.000003 | 2.285304 | | H | 2.095146 | -1.207038 | -1.477212 | | H | 3.040009 | -1.171933 | 0.015217 | | H | 3.040011 | 1.171933 | 0.015212 | | H | 2.095144 | 1.207033 | -1.477215 | | H | -1.597351 | -1.325376 | 1.194786 | | H | -2.08258 | -2.139695 | -0.29953 | | H | -2.082581 | 2.139695 | -0.299529 | | H | -1.59735 | 1.325375 | 1.194787 | | H | -2.935434 | 0 | -1.218295 | | H | -3.534778 | 0 | 0.447119 | |  |  |  |  | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.381883 | 0.748353 | -0.387131 | | C | 0.369798 | -0.777621 | -0.467491 | | C | -0.880694 | 1.149551 | 0.328404 | | C | -0.918476 | -1.124633 | 0.308762 | | C | -0.97415 | -0.001501 | 1.363299 | | C | -2.082728 | 0.817626 | -0.585587 | | C | -2.113107 | -0.74153 | -0.588011 | | C | 1.76383 | 1.237324 | -0.037018 | | C | 1.72343 | -1.174362 | 0.150477 | | C | 2.648676 | -0.008845 | -0.234208 | | H | 0.316545 | -1.152851 | -1.501128 | | H | -0.88407 | 2.166961 | 0.731442 | | H | -0.954319 | -2.150872 | 0.690278 | | H | -0.138431 | -0.013533 | 2.070142 | | H | -1.914155 | 0.006032 | 1.92833 | | H | -1.954054 | 1.24021 | -1.585569 | | H | -3.005986 | 1.229976 | -0.164757 | | H | -3.0493 | -1.115851 | -0.160616 | | H | -2.01955 | -1.163956 | -1.593385 | | H | 1.791759 | 1.566204 | 1.01458 | | H | 2.085287 | 2.094544 | -0.640614 | | H | 2.081115 | -2.146893 | -0.203274 | | H | 1.633563 | -1.230963 | 1.242334 | | H | 2.929194 | -0.097293 | -1.28999 | | H | 3.571625 | 0.022113 | 0.353247 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R5** | | | | **R6** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.350357 | -0.825491 | -0.525469 | | C | -0.398433 | 0.743945 | -0.566562 | | C | 0.872848 | -1.1191 | 0.375624 | | C | 0.822013 | 1.141064 | 0.282966 | | C | 0.81772 | 0.050663 | 1.36992 | | C | 2.139627 | -0.775111 | -0.428686 | | C | 2.098416 | 0.781631 | -0.502048 | | C | -1.684982 | -1.228276 | 0.015957 | | C | -1.758062 | 1.153083 | 0.042654 | | C | -2.65761 | -0.09339 | -0.054774 | | H | -0.186253 | -1.261127 | -1.525257 | | H | -0.308853 | 1.125432 | -1.59119 | | H | 0.869925 | -2.125335 | 0.807725 | | H | 0.792444 | 2.178 | 0.636177 | | H | -0.082924 | 0.043228 | 1.990933 | | H | 1.697528 | 0.098727 | 2.021859 | | H | 2.1393 | -1.247328 | -1.416463 | | H | 3.03548 | -1.119696 | 0.098488 | | H | 2.980972 | 1.220757 | -0.025225 | | H | 2.061376 | 1.157243 | -1.529822 | | H | -1.979126 | -2.266367 | 0.143577 | | H | -2.183917 | 2.02365 | -0.466065 | | H | -1.625182 | 1.428331 | 1.094529 | | H | -3.19027 | -0.100958 | -1.020897 | | H | -3.427575 | -0.128666 | 0.724137 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.379506 | -0.786675 | -0.582736 | | C | -0.379505 | 0.786675 | -0.582735 | | C | 0.81636 | -1.130205 | 0.32341 | | C | 0.816357 | 1.130202 | 0.323417 | | C | 0.75241 | -0.000005 | 1.365748 | | C | 2.113179 | -0.779169 | -0.428733 | | C | 2.113178 | 0.779175 | -0.428727 | | C | -1.752008 | -1.235208 | -0.03154 | | C | -1.752008 | 1.23521 | -0.031542 | | C | -2.595004 | 0.000001 | -0.015902 | | H | -0.231031 | -1.186871 | -1.592632 | | H | -0.231026 | 1.186872 | -1.59263 | | H | 0.790243 | -2.153346 | 0.714703 | | H | 0.790237 | 2.153341 | 0.714714 | | H | -0.169064 | -0.000008 | 1.957326 | | H | 1.608153 | -0.000006 | 2.050599 | | H | 2.126341 | -1.204578 | -1.437405 | | H | 2.986138 | -1.171974 | 0.103155 | | H | 2.986133 | 1.171975 | 0.103172 | | H | 2.126348 | 1.204593 | -1.437394 | | H | -1.635935 | -1.651408 | 0.983883 | | H | -2.192206 | -2.039101 | -0.634444 | | H | -2.192205 | 2.039101 | -0.634449 | | H | -1.635937 | 1.651412 | 0.98388 | | H | -3.646908 | 0.000001 | 0.253554 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **JP-10 B3LYP/def2-TZVP** | | | |  | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.36439 | -0.787455 | -0.51267 | | C | -0.36439 | 0.787456 | -0.512666 | | C | 0.883784 | -1.131549 | 0.325555 | | C | 0.88378 | 1.131545 | 0.325568 | | C | 0.894691 | -0.000008 | 1.370829 | | C | 2.135266 | -0.781168 | -0.507259 | | C | 2.135262 | 0.781178 | -0.507253 | | C | -1.724307 | -1.203612 | 0.081085 | | C | -1.724308 | 1.203613 | 0.081085 | | C | -2.641653 | 0 | -0.171254 | | H | -0.268338 | -1.185699 | -1.524931 | | H | -0.268335 | 1.185705 | -1.524925 | | H | 0.882773 | -2.149132 | 0.717323 | | H | 0.882766 | 2.149124 | 0.717344 | | H | 0.025842 | -0.000015 | 2.029763 | | H | 1.793692 | -0.000011 | 1.990989 | | H | 2.087322 | -1.20194 | -1.513055 | | H | 3.037011 | -1.172474 | -0.032878 | | H | 3.037006 | 1.172487 | -0.032873 | | H | 2.087309 | 1.201957 | -1.513046 | | H | -1.631147 | -1.372976 | 1.158043 | | H | -2.103167 | -2.129512 | -0.354984 | | H | -2.103167 | 2.129513 | -0.354984 | | H | -1.631152 | 1.372975 | 1.158043 | | H | -2.975415 | -0.000001 | -1.213824 | | H | -3.535404 | 0 | 0.455864 | | | | |  | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R1 B3LYP/def2-TZVP** | | | | **R2 B3LYP/def2-TZVP** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.355894 | 0.792306 | -0.53033 | | C | 0.306604 | -0.780814 | -0.513364 | | C | -0.907096 | 1.178281 | 0.301743 | | C | -0.949187 | -1.088092 | 0.333403 | | C | -0.92523 | 0.055858 | 1.365895 | | C | -2.097596 | 0.792575 | -0.522272 | | C | -2.197766 | -0.708812 | -0.501063 | | C | 1.721116 | 1.177706 | 0.073957 | | C | 1.653931 | -1.231267 | 0.084292 | | C | 2.605284 | -0.053424 | -0.166787 | | H | 0.276334 | 1.184366 | -1.545156 | | H | 0.196708 | -1.185292 | -1.521567 | | H | -0.89429 | 2.205176 | 0.666205 | | H | -0.973161 | -2.100444 | 0.736414 | | H | -0.045505 | 0.046901 | 2.00987 | | H | -1.815755 | 0.084477 | 1.99575 | | H | -2.587128 | 1.435708 | -1.240225 | | H | -3.116732 | -1.054329 | -0.007842 | | H | -2.192411 | -1.161513 | -1.498986 | | H | 1.624834 | 1.356524 | 1.148774 | | H | 2.127653 | 2.089546 | -0.366432 | | H | 2.009667 | -2.167152 | -0.349756 | | H | 1.553791 | -1.397251 | 1.161095 | | H | 2.945529 | -0.066824 | -1.207068 | | H | 3.494744 | -0.075796 | 0.466089 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.368517 | -0.854347 | -0.460858 | | C | -0.341361 | 0.738596 | -0.550968 | | C | 0.872674 | -1.095538 | 0.366195 | | C | 0.913538 | 1.110369 | 0.276599 | | C | 0.895574 | 0.026729 | 1.390655 | | C | 2.140003 | -0.885496 | -0.433762 | | C | 2.173488 | 0.691194 | -0.520366 | | C | -1.734572 | -1.202953 | 0.161449 | | C | -1.696414 | 1.202312 | 0.013522 | | C | -2.629862 | -0.001454 | -0.16922 | | H | -0.279869 | -1.305579 | -1.450371 | | H | -0.233917 | 1.069099 | -1.585907 | | H | 0.92566 | 2.149076 | 0.61005 | | H | 0.019796 | 0.076304 | 2.036094 | | H | 1.793027 | 0.041003 | 2.010753 | | H | 2.10369 | -1.358247 | -1.4156 | | H | 3.020351 | -1.262102 | 0.089867 | | H | 3.077083 | 1.087424 | -0.054309 | | H | 2.146395 | 1.049679 | -1.55054 | | H | -1.640726 | -1.306851 | 1.245394 | | H | -2.128498 | -2.147549 | -0.216089 | | H | -2.061705 | 2.105201 | -0.479058 | | H | -1.602869 | 1.434633 | 1.078381 | | H | -2.960412 | -0.059782 | -1.211171 | | H | -3.525309 | 0.051214 | 0.453034 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R3 B3LYP/def2-TZVP** | | | | **R4 B3LYP/def2-TZVP** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.358103 | -0.788763 | -0.494995 | | C | -0.358103 | 0.788764 | -0.494995 | | C | 0.882363 | -1.135664 | 0.362626 | | C | 0.882365 | 1.135667 | 0.362621 | | C | 0.887008 | 0.000004 | 1.350522 | | C | 2.148681 | -0.782213 | -0.471695 | | C | 2.148682 | 0.782208 | -0.471699 | | C | -1.716346 | -1.199953 | 0.102585 | | C | -1.716345 | 1.199953 | 0.102587 | | C | -2.633868 | 0 | -0.161136 | | H | -0.254746 | -1.189646 | -1.505502 | | H | -0.254749 | 1.189645 | -1.505503 | | H | 0.881376 | -2.148915 | 0.761614 | | H | 0.88138 | 2.14892 | 0.761605 | | H | 1.35877 | 0.000005 | 2.323897 | | H | 2.101446 | -1.205294 | -1.477385 | | H | 3.046368 | -1.17361 | 0.008706 | | H | 3.046371 | 1.173607 | 0.008696 | | H | 2.101444 | 1.205284 | -1.477392 | | H | -1.612759 | -1.344406 | 1.182348 | | H | -2.094332 | -2.133664 | -0.3176 | | H | -2.094332 | 2.133664 | -0.317596 | | H | -1.612757 | 1.344403 | 1.18235 | | H | -2.959549 | 0 | -1.206498 | | H | -3.531949 | 0 | 0.459732 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.385824 | 0.745625 | -0.365345 | | C | 0.372843 | -0.773608 | -0.464913 | | C | -0.880309 | 1.146474 | 0.336827 | | C | -0.926054 | -1.128023 | 0.300251 | | C | -0.987893 | -0.014985 | 1.368513 | | C | -2.085515 | 0.825678 | -0.583361 | | C | -2.117932 | -0.735877 | -0.600806 | | C | 1.76521 | 1.242531 | -0.049022 | | C | 1.73113 | -1.180532 | 0.141465 | | C | 2.657751 | -0.006354 | -0.221753 | | H | 0.319488 | -1.135781 | -1.498856 | | H | -0.883555 | 2.156134 | 0.745546 | | H | -0.964676 | -2.153518 | 0.667466 | | H | -0.159321 | -0.035145 | 2.077982 | | H | -1.926855 | -0.008136 | 1.927694 | | H | -1.958705 | 1.255107 | -1.576961 | | H | -3.005279 | 1.23368 | -0.15967 | | H | -3.054104 | -1.112089 | -0.184484 | | H | -2.020476 | -1.145441 | -1.607364 | | H | 1.805892 | 1.603381 | 0.989833 | | H | 2.087032 | 2.082398 | -0.672779 | | H | 2.092798 | -2.14166 | -0.228297 | | H | 1.64549 | -1.259663 | 1.229452 | | H | 2.968664 | -0.094355 | -1.266524 | | H | 3.563279 | 0.029505 | 0.385822 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **R5 B3LYP/def2-TZVP** | | | | **R6 B3LYP/def2-TZVP** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.355427 | -0.823585 | -0.529747 | | C | -0.39841 | 0.748529 | -0.567637 | | C | 0.8734 | -1.119914 | 0.373906 | | C | 0.825336 | 1.139828 | 0.287563 | | C | 0.820626 | 0.047198 | 1.374375 | | C | 2.144451 | -0.776252 | -0.428893 | | C | 2.106506 | 0.783674 | -0.496387 | | C | -1.689329 | -1.230022 | -0.013332 | | C | -1.767002 | 1.158835 | 0.025443 | | C | -2.658486 | -0.099741 | -0.030847 | | H | -0.178314 | -1.25631 | -1.524508 | | H | -0.298134 | 1.128373 | -1.585926 | | H | 0.868701 | -2.123212 | 0.798886 | | H | 0.79613 | 2.170965 | 0.640977 | | H | -0.077847 | 0.041974 | 1.992873 | | H | 1.694091 | 0.091691 | 2.028377 | | H | 2.144442 | -1.241662 | -1.416099 | | H | 3.036369 | -1.124216 | 0.095287 | | H | 2.985476 | 1.218378 | -0.017236 | | H | 2.074651 | 1.159298 | -1.520637 | | H | -1.968701 | -2.260775 | 0.163574 | | H | -2.205462 | 2.004017 | -0.507062 | | H | -1.643534 | 1.469367 | 1.065365 | | H | -3.248335 | -0.107939 | -0.962671 | | H | -3.389528 | -0.141246 | 0.782137 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.380728 | -0.78775 | -0.583878 | | C | -0.380728 | 0.787747 | -0.583882 | | C | 0.818025 | -1.129842 | 0.325012 | | C | 0.818027 | 1.129846 | 0.325005 | | C | 0.756104 | 0.000006 | 1.370958 | | C | 2.118718 | -0.780583 | -0.426884 | | C | 2.118725 | 0.780575 | -0.426879 | | C | -1.761282 | -1.23654 | -0.049169 | | C | -1.761282 | 1.23654 | -0.049176 | | C | -2.585004 | 0 | 0.032446 | | H | -0.225482 | -1.186497 | -1.587341 | | H | -0.225483 | 1.186489 | -1.587347 | | H | 0.792548 | -2.148399 | 0.713103 | | H | 0.792553 | 2.148405 | 0.713089 | | H | -0.162351 | 0.000011 | 1.960684 | | H | 1.606275 | 0.000008 | 2.056361 | | H | 2.13352 | -1.202238 | -1.433342 | | H | 2.988333 | -1.172829 | 0.103429 | | H | 2.988342 | 1.172811 | 0.10344 | | H | 2.133537 | 1.202233 | -1.433335 | | H | -1.654937 | -1.711308 | 0.93963 | | H | -2.218658 | -2.002384 | -0.685553 | | H | -2.218658 | 2.00238 | -0.685565 | | H | -1.654937 | 1.711313 | 0.93962 | | H | -3.638055 | 0 | 0.281804 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 sites 1-2 JP-10/AlO** | | | | **vdW1 site 3 JP-10/AlO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -1.845897 | -0.620373 | 0.222476 | | C | -1.155568 | 0.139051 | -0.966474 | | C | -0.657847 | -1.261778 | 0.958818 | | C | 0.336887 | -0.164876 | -0.752322 | | C | 0.441198 | -0.195486 | 0.785574 | | C | -0.102931 | -2.400434 | 0.081327 | | C | 0.591991 | -1.644321 | -1.091889 | | C | -2.621317 | 0.455373 | 1.005694 | | C | -1.568272 | 1.614827 | -0.811679 | | C | -2.883426 | 1.55969 | -0.025263 | | H | -2.539274 | -1.390332 | -0.139299 | | H | -1.490872 | -0.242427 | -1.939263 | | H | -0.879792 | -1.556137 | 1.990638 | | H | 0.997202 | 0.529158 | -1.287133 | | H | 0.208346 | 0.756472 | 1.274112 | | H | 1.411559 | -0.558918 | 1.145346 | | H | -0.897247 | -3.073353 | -0.257415 | | H | 0.621199 | -3.001337 | 0.640958 | | H | 1.666924 | -1.847015 | -1.108146 | | H | 0.183701 | -1.911525 | -2.071848 | | H | -2.002528 | 0.850581 | 1.820965 | | H | -3.535386 | 0.057114 | 1.457996 | | H | -1.660507 | 2.121025 | -1.778144 | | H | -0.813483 | 2.160882 | -0.231675 | | H | -3.700804 | 1.258237 | -0.691517 | | H | -3.159462 | 2.518372 | 0.426088 | | Al | 3.328476 | 1.550786 | 0.265866 | | O | 3.638917 | -0.215132 | 0.106815 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 1.094905 | 0.865603 | -0.785911 | | C | 1.094954 | 0.86567 | 0.785849 | | C | 1.418394 | -0.598591 | -1.129651 | | C | 1.418461 | -0.598445 | 1.129697 | | C | 0.697759 | -1.35731 | 0.000094 | | C | 2.897022 | -0.854888 | -0.779781 | | C | 2.897088 | -0.854783 | 0.779727 | | C | -0.307657 | 1.352815 | -1.193689 | | C | -0.30763 | 1.352927 | 1.193644 | | C | -0.772774 | 2.194939 | -0.000063 | | H | 1.86182 | 1.541789 | -1.188571 | | H | 1.861837 | 1.541958 | 1.188402 | | H | 1.145022 | -0.881994 | -2.153021 | | H | 1.145236 | -0.881835 | 2.153111 | | H | -0.388584 | -1.236181 | 0.00013 | | H | 0.94209 | -2.428048 | 0.000166 | | H | 3.558086 | -0.09098 | -1.203832 | | H | 3.22442 | -1.824595 | -1.171292 | | H | 3.224488 | -1.824443 | 1.171351 | | H | 3.558166 | -0.090816 | 1.203637 | | H | -0.987552 | 0.501466 | -1.293879 | | H | -0.291579 | 1.904081 | -2.141517 | | H | -0.291498 | 1.904308 | 2.141399 | | H | -0.987503 | 0.501595 | 1.29398 | | H | -0.271678 | 3.172442 | -0.000097 | | H | -1.854736 | 2.369116 | -0.00003 | | Al | -4.219396 | -0.900399 | -0.000009 | | O | -2.672378 | -0.835037 | 0.000085 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 site 4 JP-10/AlO** | | | | **vdW1 sites 5-6 JP-10/AlO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.665171 | 0.357543 | 0.784778 | | C | 0.665205 | 0.357554 | -0.784777 | | C | 0.912678 | -1.121426 | 1.130932 | | C | 0.912668 | -1.121412 | -1.130933 | | C | 1.857914 | -1.565132 | -0.00001 | | C | -0.365245 | -1.908466 | 0.778975 | | C | -0.365315 | -1.908384 | -0.778949 | | C | 1.777072 | 1.338172 | 1.199812 | | C | 1.777167 | 1.338165 | -1.199739 | | C | 1.911507 | 2.284429 | 0.000037 | | H | -0.307568 | 0.691771 | 1.158514 | | H | -0.307488 | 0.691877 | -1.158554 | | H | 1.273122 | -1.285785 | 2.15384 | | H | 1.273076 | -1.285804 | -2.153848 | | H | 2.822474 | -1.047768 | -0.000016 | | H | 2.043222 | -2.646375 | -0.000018 | | H | -1.259169 | -1.424885 | 1.179056 | | H | -0.3114 | -2.928887 | 1.177378 | | H | -0.311632 | -2.928762 | -1.177467 | | H | -1.259203 | -1.42461 | -1.178874 | | H | 2.723101 | 0.802899 | 1.35425 | | H | 1.542938 | 1.857442 | 2.135851 | | H | 1.543087 | 1.85743 | -2.135794 | | H | 2.72321 | 0.802897 | -1.354106 | | H | 1.078668 | 2.998295 | 0 | | H | 2.844591 | 2.859499 | 0.000071 | | Al | -4.166579 | 0.716618 | 0.000167 | | O | -2.554806 | 0.59856 | -0.000402 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.374399 | 0.225682 | 0.784799 | | C | 0.374378 | 0.22567 | -0.784776 | | C | 1.763555 | -0.336618 | 1.131767 | | C | 1.763558 | -0.336612 | -1.131748 | | C | 2.636416 | 0.235031 | 0.000013 | | C | 1.76887 | -1.836983 | 0.779783 | | C | 1.768903 | -1.836966 | -0.779809 | | C | 0.114403 | 1.685441 | 1.198245 | | C | 0.114387 | 1.68541 | -1.198241 | | C | -0.631229 | 2.284209 | 0.000004 | | H | -0.430733 | -0.409704 | 1.166424 | | H | -0.430734 | -0.40974 | -1.166379 | | H | 2.093661 | -0.117393 | 2.154157 | | H | 2.093646 | -0.117339 | -2.154134 | | H | 2.696645 | 1.327245 | 0.00002 | | H | 3.655761 | -0.170354 | 0.000015 | | H | 0.901744 | -2.354158 | 1.20369 | | H | 2.667964 | -2.325892 | 1.171656 | | H | 2.66805 | -2.325818 | -1.171635 | | H | 0.901837 | -2.354197 | -1.203768 | | H | 1.064672 | 2.214131 | 1.354065 | | H | -0.452031 | 1.750104 | 2.133644 | | H | -0.452064 | 1.750079 | -2.133623 | | H | 1.064656 | 2.214088 | -1.354078 | | H | -1.65978 | 1.912552 | -0.000001 | | H | -0.644884 | 3.380763 | -0.000023 | | Al | -4.12735 | -1.111835 | 0.000055 | | O | -2.796088 | -0.184513 | -0.00012 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS1 JP-10/AlO** | | | | **TS2 JP-10/AlO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.116564 | -0.655207 | 0.663072 | | C | 1.802351 | 0.729226 | 0.378115 | | C | -0.259943 | -0.506549 | -0.014586 | | C | 0.720156 | 1.495932 | -0.401738 | | C | 0.06467 | 0.377051 | -1.23166 | | C | -1.085295 | 0.469326 | 0.826796 | | C | -0.413142 | 1.843793 | 0.584734 | | C | 2.047301 | -1.715498 | 0.043943 | | C | 3.090234 | 0.399492 | -0.398814 | | C | 3.42312 | -1.039077 | 0.014456 | | H | 1.005074 | -0.838427 | 1.73951 | | H | 2.055022 | 1.251551 | 1.309739 | | H | -0.754045 | -1.46255 | -0.223745 | | H | 1.099307 | 2.356105 | -0.964233 | | H | 0.741049 | -0.093553 | -1.950479 | | H | -0.838832 | 0.706018 | -1.754623 | | H | -1.206764 | 0.18254 | 1.876206 | | H | -2.156302 | 0.543751 | 0.375681 | | H | -1.123485 | 2.545609 | 0.136274 | | H | -0.034412 | 2.294727 | 1.507817 | | H | 1.727484 | -1.946646 | -0.979579 | | H | 2.035656 | -2.654143 | 0.607232 | | H | 3.894173 | 1.110474 | -0.182791 | | H | 2.902877 | 0.440044 | -1.478769 | | H | 3.860329 | -1.044114 | 1.020287 | | H | 4.132985 | -1.530992 | -0.658618 | | Al | -4.100233 | -1.089066 | -0.030696 | | O | -3.384149 | 0.488316 | -0.345846 | | | | | |  |  |  |  | | --- | --- | --- | --- | | Al | 4.359131 | -0.373861 | 0.151823 | | C | -0.548599 | -0.404625 | -0.785763 | | C | -2.005954 | -0.145166 | -0.243774 | | C | 0.24915 | 0.717371 | -0.11765 | | C | -1.826592 | 1.093828 | 0.653966 | | C | -0.425805 | 0.85305 | 1.252053 | | C | -0.104063 | 2.053387 | -0.779919 | | C | -1.554762 | 2.31116 | -0.254639 | | C | -0.191037 | -1.836072 | -0.348234 | | C | -2.412091 | -1.444405 | 0.476954 | | C | -1.547769 | -2.529467 | -0.177181 | | H | -0.500966 | -0.320255 | -1.87866 | | H | -2.707421 | 0.063726 | -1.06194 | | H | 1.392976 | 0.487391 | -0.084981 | | H | -2.642549 | 1.244229 | 1.370641 | | H | -0.353345 | -0.04366 | 1.872937 | | H | -0.052647 | 1.708771 | 1.825371 | | H | -0.048411 | 1.997422 | -1.871404 | | H | 0.580359 | 2.842184 | -0.451711 | | H | -1.601872 | 3.241279 | 0.321697 | | H | -2.289207 | 2.387657 | -1.063189 | | H | 0.346214 | -1.811443 | 0.606663 | | H | 0.466141 | -2.329638 | -1.07088 | | H | -3.48696 | -1.639164 | 0.399101 | | H | -2.171833 | -1.374885 | 1.54499 | | H | -1.95988 | -2.787048 | -1.16069 | | H | -1.493293 | -3.451866 | 0.410987 | | O | 2.757389 | 0.078891 | 0.032811 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS3 JP-10/AlO** | | | | **TS4 JP-10/AlO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.049354 | 0.881022 | -0.785793 | | C | 1.049191 | 0.880943 | 0.785963 | | C | 1.181733 | -0.611337 | -1.135446 | | C | 1.181587 | -0.611449 | 1.135446 | | C | 0.409667 | -1.289585 | -0.000086 | | C | 2.619517 | -1.053605 | -0.78053 | | C | 2.619473 | -1.05352 | 0.780627 | | C | -0.273364 | 1.552272 | -1.198781 | | C | -0.273623 | 1.552117 | 1.198756 | | C | -0.635485 | 2.43752 | 0.000006 | | H | 1.899487 | 1.448272 | -1.186898 | | H | 1.899214 | 1.448198 | 1.187295 | | H | 0.871641 | -0.865458 | -2.154516 | | H | 0.871414 | -0.865735 | 2.15445 | | H | -0.750295 | -1.067259 | -0.000128 | | H | 0.468856 | -2.38491 | -0.000149 | | H | 3.36656 | -0.375137 | -1.205997 | | H | 2.823256 | -2.055487 | -1.172413 | | H | 2.823464 | -2.055287 | 1.172671 | | H | 3.366319 | -0.374793 | 1.206025 | | H | -1.047711 | 0.791467 | -1.332078 | | H | -0.177111 | 2.107535 | -2.138111 | | H | -0.177571 | 2.107256 | 2.13818 | | H | -1.047992 | 0.791291 | 1.331785 | | H | -0.015482 | 3.342995 | 0.000132 | | H | -1.684557 | 2.75434 | -0.000091 | | Al | -3.82982 | -0.95691 | 0.000036 | | O | -2.158767 | -1.051718 | -0.000199 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.155667 | 0.3486 | 0.505311 | | C | 0.853518 | 0.378237 | -0.891863 | | C | 0.764756 | -0.876448 | 1.193412 | | C | 1.804295 | -0.830742 | -0.82097 | | C | 2.212993 | -0.832689 | 0.663428 | | C | 0.22272 | -2.135075 | 0.48736 | | C | 0.947268 | -2.109532 | -0.892939 | | C | 0.397304 | 1.721078 | 1.143645 | | C | 1.509325 | 1.768156 | -0.983183 | | C | 0.657211 | 2.642763 | -0.054213 | | H | -0.97904 | 0.206681 | 0.369911 | | H | 0.123228 | 0.256281 | -1.701825 | | H | 0.644528 | -0.882989 | 2.282302 | | H | 2.623218 | -0.798137 | -1.548967 | | H | 2.767446 | 0.058809 | 0.972009 | | H | 2.793657 | -1.719728 | 0.943942 | | H | -0.865033 | -2.092346 | 0.394745 | | H | 0.482922 | -3.037276 | 1.051776 | | H | 1.583646 | -2.99221 | -1.020101 | | H | 0.248535 | -2.083338 | -1.735341 | | H | 1.286007 | 1.685953 | 1.789457 | | H | -0.446707 | 2.038104 | 1.764581 | | H | 1.55156 | 2.139276 | -2.012765 | | H | 2.540071 | 1.726268 | -0.608853 | | H | -0.294981 | 2.880901 | -0.542901 | | H | 1.140844 | 3.586861 | 0.21901 | | Al | -4.063433 | -0.134438 | -0.253408 | | O | -2.440701 | 0.041061 | 0.072175 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS5 JP-10/AlO** | | | | **TS6 JP-10/AlO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.020121 | 0.050079 | -0.349404 | | C | 1.340017 | 0.872062 | -0.588349 | | C | 0.50375 | -1.149724 | 0.483128 | | C | 2.403076 | 0.032033 | 0.140718 | | C | 1.611775 | -0.515369 | 1.341925 | | C | 1.325824 | -2.06745 | -0.441635 | | C | 2.636201 | -1.254735 | -0.673887 | | C | -0.927217 | 1.018915 | 0.362575 | | C | 1.071672 | 2.270156 | 0.001992 | | C | -0.457408 | 2.417176 | -0.029266 | | H | -0.431221 | -0.274711 | -1.294879 | | H | 1.571388 | 0.955695 | -1.65749 | | H | -0.292114 | -1.66834 | 1.031526 | | H | 3.318878 | 0.585523 | 0.376283 | | H | 1.252078 | 0.259308 | 2.025864 | | H | 2.175899 | -1.255509 | 1.920506 | | H | 0.792889 | -2.289723 | -1.371566 | | H | 1.537519 | -3.021861 | 0.051266 | | H | 3.506946 | -1.799027 | -0.293883 | | H | 2.820444 | -1.039474 | -1.731179 | | H | -0.946449 | 0.87409 | 1.449022 | | H | -2.027036 | 0.855289 | -0.005625 | | H | 1.588158 | 3.058554 | -0.555025 | | H | 1.427016 | 2.317903 | 1.038364 | | H | -0.791287 | 2.640835 | -1.048698 | | H | -0.837812 | 3.20276 | 0.630031 | | Al | -3.526499 | -1.257558 | 0.137845 | | O | -3.24846 | 0.363509 | -0.480411 | | | | | |  |  |  |  | | --- | --- | --- | --- | | Al | 5.233121 | -0.000056 | -0.236816 | | C | -0.904529 | 0.78603 | -0.620168 | | C | -0.904495 | -0.78603 | -0.620033 | | C | -2.108321 | 1.128406 | 0.279118 | | C | -2.108135 | -1.128326 | 0.279502 | | C | -2.083838 | 0.000218 | 1.324306 | | C | -3.39188 | 0.779333 | -0.498987 | | C | -3.391819 | -0.77976 | -0.498609 | | C | 0.473292 | 1.21582 | -0.068559 | | C | 0.47347 | -1.215654 | -0.068697 | | C | 1.055739 | 0.000082 | 0.652848 | | H | -1.058132 | 1.19858 | -1.625128 | | H | -1.058302 | -1.198748 | -1.624893 | | H | -2.089052 | 2.152894 | 0.667544 | | H | -2.088637 | -2.152678 | 0.668273 | | H | -1.197566 | 0.0004 | 1.96182 | | H | -2.974603 | 0.000245 | 1.964035 | | H | -3.385766 | 1.203874 | -1.508078 | | H | -4.274245 | 1.173206 | 0.016606 | | H | -4.274072 | -1.173437 | 0.017329 | | H | -3.385839 | -1.204805 | -1.507488 | | H | 0.401857 | 2.099578 | 0.575449 | | H | 1.132124 | 1.477666 | -0.904439 | | H | 1.132238 | -1.477162 | -0.904735 | | H | 0.402355 | -2.099573 | 0.575125 | | H | 2.213322 | 0.00013 | 0.545813 | | H | 0.871088 | 0.000024 | 1.731274 | | O | 3.618218 | -0.000023 | 0.183222 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 JP-10/R1** | | | | **vdW2 JP-10/R2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.63335 | -0.51238 | 0.808329 | | C | 1.862562 | 0.875495 | 0.108984 | | C | 0.132283 | -0.795691 | 0.519682 | | C | 0.481968 | 1.20241 | -0.49301 | | C | -0.030362 | -0.193318 | -0.891683 | | C | -0.637124 | 0.203396 | 1.338856 | | C | -0.474411 | 1.550599 | 0.668824 | | C | 2.633737 | -1.483462 | 0.152321 | | C | 2.994568 | 0.640793 | -0.908536 | | C | 3.756118 | -0.571905 | -0.359314 | | H | 1.81814 | -0.457129 | 1.887961 | | H | 2.164553 | 1.643809 | 0.832121 | | H | -0.156394 | -1.843527 | 0.651866 | | H | 0.508821 | 1.952717 | -1.290318 | | H | 0.583784 | -0.68679 | -1.649704 | | H | -1.071172 | -0.186587 | -1.226731 | | H | -0.816588 | 0.081283 | 2.404653 | | H | -2.665978 | -0.126502 | 0.538375 | | H | -1.432064 | 1.928718 | 0.283161 | | H | -0.069012 | 2.32003 | 1.337799 | | H | 2.163178 | -2.002129 | -0.691572 | | H | 2.981397 | -2.250161 | 0.852086 | | H | 3.624802 | 1.526949 | -1.035111 | | H | 2.574628 | 0.398878 | -1.892552 | | H | 4.391779 | -0.261909 | 0.478938 | | H | 4.399594 | -1.053192 | -1.103238 | | Al | -5.044944 | -0.439893 | -0.448413 | | O | -3.441417 | -0.095185 | -0.026884 | | | | | |  |  |  |  | | --- | --- | --- | --- | | Al | 4.51426 | 0.017514 | 0.151504 | | C | -0.765515 | -0.382176 | -0.960334 | | C | -1.997021 | -0.457327 | 0.04067 | | C | -0.132211 | 0.911417 | -0.498812 | | C | -1.823516 | 0.806745 | 0.910961 | | C | -0.281742 | 0.910097 | 1.016267 | | C | -0.925196 | 2.122866 | -0.943274 | | C | -2.146213 | 2.046433 | 0.045553 | | C | 0.025654 | -1.684586 | -0.734965 | | C | -1.840484 | -1.80197 | 0.773014 | | C | -1.015603 | -2.667495 | -0.186336 | | H | -1.100482 | -0.311698 | -2.001755 | | H | -2.949547 | -0.431001 | -0.503528 | | H | -2.373238 | 0.768289 | 1.858431 | | H | 0.193528 | 0.065584 | 1.517824 | | H | 0.054431 | 1.839641 | 1.48598 | | H | -1.223759 | 2.065169 | -1.993417 | | H | -0.363069 | 3.050633 | -0.798927 | | H | -2.201516 | 2.947873 | 0.664223 | | H | -3.101353 | 1.943999 | -0.47896 | | H | 0.822374 | -1.525147 | -0.001692 | | H | 0.504181 | -2.030238 | -1.656688 | | H | -2.809624 | -2.241565 | 1.03076 | | H | -1.288075 | -1.660176 | 1.70973 | | H | -1.653954 | -3.028678 | -1.001914 | | H | -0.568712 | -3.541937 | 0.297648 | | O | 2.8453 | 0.302666 | 0.16759 | | H | 2.022119 | 0.616211 | -0.214443 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 JP-10/R3** | | | | **vdW2 JP-10/R4** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | Al | 4.095524 | -0.69772 | -0.000129 | | C | -1.088607 | 0.887382 | 0.786423 | | C | -1.087972 | 0.886736 | -0.787095 | | C | -1.379 | -0.584568 | 1.138781 | | C | -1.377783 | -0.585652 | -1.138361 | | C | -0.699266 | -1.310212 | 0.000885 | | C | -2.861715 | -0.871703 | 0.780555 | | C | -2.860897 | -0.872419 | -0.781416 | | C | 0.305547 | 1.395537 | 1.195541 | | C | 0.306204 | 1.395255 | -1.195751 | | C | 0.768171 | 2.235265 | -0.000031 | | H | -1.867297 | 1.545808 | 1.191469 | | H | -1.86677 | 1.544285 | -1.193337 | | H | -1.097301 | -0.872298 | 2.155848 | | H | -1.094942 | -0.874355 | -2.154832 | | H | -0.514711 | -2.384328 | 0.001415 | | H | -3.529249 | -0.115547 | 1.206827 | | H | -3.171417 | -1.84535 | 1.172437 | | H | -3.170353 | -1.846368 | -1.172744 | | H | -3.527907 | -0.116581 | -1.209065 | | H | 0.984735 | 0.545272 | 1.321992 | | H | 0.286597 | 1.947269 | 2.140998 | | H | 0.287188 | 1.947224 | -2.141062 | | H | 0.985684 | 0.545213 | -1.322272 | | H | 0.255492 | 3.205005 | -0.000355 | | H | 1.846117 | 2.429943 | 0.000291 | | O | 2.5291 | -1.342602 | 0.000644 | | H | 1.57142 | -1.297743 | 0.001731 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.430832 | 0.376646 | 0.635545 | | C | 0.786479 | 0.379587 | -0.852382 | | C | 1.030918 | -0.872995 | 1.223273 | | C | 1.657814 | -0.888466 | -0.964546 | | C | 2.35191 | -0.928228 | 0.411189 | | C | 0.285709 | -2.09836 | 0.644126 | | C | 0.71297 | -2.103384 | -0.85505 | | C | 0.580955 | 1.763759 | 1.207038 | | C | 1.45139 | 1.754653 | -1.048029 | | C | 0.712478 | 2.65329 | -0.043653 | | H | -1.633192 | 0.132118 | 0.231936 | | H | -0.0972 | 0.307527 | -1.502862 | | H | 1.129034 | -0.872016 | 2.313182 | | H | 2.315742 | -0.907387 | -1.839944 | | H | 3.012134 | -0.076078 | 0.601445 | | H | 2.913338 | -1.854801 | 0.580693 | | H | -0.79604 | -2.016299 | 0.769966 | | H | 0.614111 | -3.010637 | 1.153174 | | H | 1.242461 | -3.027258 | -1.10989 | | H | -0.143269 | -2.014138 | -1.530201 | | H | 1.497296 | 1.814299 | 1.817067 | | H | -0.247031 | 2.056055 | 1.864232 | | H | 1.380745 | 2.110769 | -2.080704 | | H | 2.51522 | 1.700133 | -0.786139 | | H | -0.285066 | 2.889969 | -0.430898 | | H | 1.227481 | 3.598333 | 0.154087 | | Al | -4.199599 | -0.066018 | -0.095101 | | O | -2.507463 | -0.023921 | -0.139237 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 JP-10/R5** | | | | **vdW2 JP-10/R6** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | Al | -4.290743 | -1.127192 | -0.247615 | | C | 0.270918 | -0.031515 | 0.617712 | | C | 0.601366 | 0.346557 | -0.868319 | | C | 1.63325 | -0.513924 | 1.177344 | | C | 2.083795 | -0.047785 | -0.989595 | | C | 2.627245 | 0.355712 | 0.393559 | | C | 1.907787 | -1.903365 | 0.575169 | | C | 2.189179 | -1.584323 | -0.924588 | | C | -0.283501 | 1.222935 | 1.213093 | | C | 0.348189 | 1.865342 | -1.007505 | | C | -0.538079 | 2.282102 | 0.184549 | | H | -0.452621 | -0.859384 | 0.674577 | | H | -0.026535 | -0.212149 | -1.57203 | | H | 1.702099 | -0.47122 | 2.269488 | | H | 2.585746 | 0.397193 | -1.856026 | | H | 2.534836 | 1.423371 | 0.614731 | | H | 3.669562 | 0.052976 | 0.545816 | | H | 1.063239 | -2.586025 | 0.714076 | | H | 2.781716 | -2.361704 | 1.049936 | | H | 3.191057 | -1.915956 | -1.216206 | | H | 1.475511 | -2.065552 | -1.60109 | | H | -0.494285 | 1.340434 | 2.272854 | | H | -2.340756 | 0.309184 | 0.671533 | | H | 1.30062 | 2.404305 | -0.967878 | | H | -1.596105 | 2.296382 | -0.118857 | | H | -0.30956 | 3.290211 | 0.549702 | | O | -3.02891 | -0.055467 | 0.116179 | | H | -0.114484 | 2.104754 | -1.969581 | | | | | |  |  |  |  | | --- | --- | --- | --- | | Al | -4.292772 | -1.099693 | -0.000807 | | C | 0.397964 | 0.082639 | 0.786753 | | C | 0.396683 | 0.080381 | -0.785972 | | C | 1.877341 | -0.164207 | 1.129895 | | C | 1.875496 | -0.167448 | -1.130826 | | C | 2.59365 | 0.593325 | -0.002137 | | C | 2.214909 | -1.625428 | 0.780591 | | C | 2.213631 | -1.627662 | -0.777889 | | C | -0.143666 | 1.45926 | 1.232616 | | C | -0.145662 | 1.455722 | -1.234909 | | C | -0.727353 | 2.074559 | -0.00156 | | H | -0.242706 | -0.713057 | 1.180435 | | H | -0.244608 | -0.71646 | -1.176319 | | H | 2.145919 | 0.123632 | 2.152527 | | H | 2.142402 | 0.117459 | -2.154716 | | H | 2.396382 | 1.670702 | -0.003517 | | H | 3.678528 | 0.437421 | -0.002801 | | H | 1.487169 | -2.322999 | 1.207143 | | H | 3.200119 | -1.89846 | 1.173063 | | H | 3.198194 | -1.901824 | -1.171197 | | H | 1.485192 | -2.326451 | -1.201246 | | H | 0.674319 | 2.086163 | 1.626705 | | H | -0.871891 | 1.369643 | 2.048088 | | H | -0.875183 | 1.363794 | -2.04897 | | H | 0.671696 | 2.081475 | -1.632113 | | H | -1.21408 | 3.047061 | -0.00256 | | O | -2.852151 | -0.210196 | 0.004287 | | H | -2.32617 | 0.592633 | 0.002295 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 Site 1 JP-10/BO** | | | | **vdW1 Site 2 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -1.286342 | -0.786229 | -0.500869 | | C | -1.286011 | 0.785302 | -0.502464 | | C | 0.148561 | -1.131535 | -0.06581 | | C | 0.149023 | 1.130911 | -0.068073 | | C | 0.468168 | 0.000617 | 0.92678 | | C | 1.098476 | -0.781059 | -1.227126 | | C | 1.098865 | 0.777729 | -1.228635 | | C | -2.40296 | -1.198466 | 0.476515 | | C | -2.402473 | 1.199985 | 0.47406 | | C | -3.358119 | 0.000968 | 0.489536 | | H | -1.498827 | -1.190246 | -1.499225 | | H | -1.498315 | 1.187373 | -1.501643 | | H | 0.263197 | -2.153772 | 0.312784 | | H | 0.264065 | 2.153855 | 0.308485 | | H | -0.168294 | 0.001641 | 1.816957 | | H | 1.517319 | 0.000729 | 1.238689 | | H | 0.756809 | -1.208964 | -2.175669 | | H | 2.104136 | -1.163338 | -1.02867 | | H | 2.104705 | 1.1599 | -1.030842 | | H | 0.757475 | 1.203941 | -2.178032 | | H | -1.988366 | -1.350936 | 1.480711 | | H | -2.886069 | -2.135383 | 0.179918 | | H | -2.885201 | 2.136491 | 0.175553 | | H | -1.987816 | 1.354335 | 1.477941 | | H | -3.966171 | 0.000156 | -0.42348 | | H | -4.042879 | 0.00198 | 1.344385 | | B | 5.330651 | 0.001592 | 0.823605 | | O | 4.142231 | 0.000618 | 0.592579 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.088229 | -0.301962 | -0.772602 | | C | -1.537642 | -0.633887 | -0.264029 | | C | 0.229213 | 1.034954 | -0.079758 | | C | -1.862899 | 0.559166 | 0.651504 | | C | -0.48917 | 0.870544 | 1.271403 | | C | -0.63346 | 2.127191 | -0.740032 | | C | -2.073633 | 1.798961 | -0.239057 | | C | 0.784279 | -1.497705 | -0.347518 | | C | -1.428503 | -2.004235 | 0.430589 | | C | -0.205062 | -2.661997 | -0.219328 | | H | -0.059714 | -0.190731 | -1.864328 | | H | -2.2538 | -0.694355 | -1.093826 | | H | 1.298561 | 1.260411 | -0.035613 | | H | -2.68191 | 0.368736 | 1.354639 | | H | -0.087696 | 0.062241 | 1.889512 | | H | -0.490971 | 1.792087 | 1.865269 | | H | -0.549549 | 2.108336 | -1.83161 | | H | -0.319238 | 3.12161 | -0.40535 | | H | -2.484583 | 2.628792 | 0.345929 | | H | -2.773151 | 1.597961 | -1.057153 | | H | 1.253237 | -1.295036 | 0.622632 | | H | 1.594264 | -1.687357 | -1.059009 | | H | -2.345631 | -2.593702 | 0.32729 | | H | -1.248385 | -1.870349 | 1.50446 | | H | -0.471591 | -3.03429 | -1.216281 | | H | 0.189167 | -3.506935 | 0.355611 | | B | 4.975952 | 0.313481 | 0.215318 | | O | 3.797735 | 0.577375 | 0.134276 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 Site 3 JP-10/BO** | | | | **vdW1 Site 4 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.637902 | 0.879564 | -0.785759 | | C | 0.637879 | 0.879491 | 0.785824 | | C | 1.139565 | -0.533352 | -1.131277 | | C | 1.139535 | -0.533457 | 1.13124 | | C | 0.524033 | -1.37646 | -0.000063 | | C | 2.637861 | -0.607415 | -0.779689 | | C | 2.637834 | -0.607533 | 0.779686 | | C | -0.811963 | 1.194611 | -1.198703 | | C | -0.812002 | 1.194486 | 1.198747 | | C | -1.392189 | 1.954425 | 0.000052 | | H | 1.315887 | 1.643402 | -1.188582 | | H | 1.315853 | 1.64329 | 1.188739 | | H | 0.903344 | -0.849141 | -2.153881 | | H | 0.903274 | -0.849327 | 2.15381 | | H | -0.56872 | -1.389443 | -0.000073 | | H | 0.888036 | -2.410971 | -0.000101 | | H | 3.198463 | 0.231959 | -1.204142 | | H | 3.081582 | -1.528928 | -1.171678 | | H | 3.081484 | -1.529141 | 1.171537 | | H | 3.198484 | 0.231732 | 1.204288 | | H | -1.375131 | 0.265998 | -1.342899 | | H | -0.858888 | 1.759385 | -2.136038 | | H | -0.858971 | 1.759157 | 2.136141 | | H | -1.375164 | 0.265849 | 1.34282 | | H | -1.02755 | 2.989375 | 0.00011 | | H | -2.486873 | 1.984457 | 0.000034 | | B | -4.336747 | -1.726171 | -0.00014 | | O | -3.210262 | -1.281621 | 0.000034 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.379974 | 0.333007 | 0.785312 | | C | 0.379837 | 0.333122 | -0.785227 | | C | 0.331391 | -1.165736 | 1.131349 | | C | 0.331193 | -1.16558 | -1.131472 | | C | 1.171149 | -1.784644 | -0.000182 | | C | -1.074783 | -1.689172 | 0.779331 | | C | -1.074915 | -1.689074 | -0.779284 | | C | 1.663274 | 1.076766 | 1.199455 | | C | 1.663058 | 1.076937 | -1.199488 | | C | 1.981561 | 1.977751 | 0.000021 | | H | -0.501502 | 0.853022 | 1.178088 | | H | -0.501717 | 0.853179 | -1.177772 | | H | 0.652307 | -1.396038 | 2.153884 | | H | 0.651931 | -1.395722 | -2.154099 | | H | 2.21806 | -1.46682 | -0.000252 | | H | 1.141007 | -2.880617 | -0.000252 | | H | -1.861519 | -1.052786 | 1.19445 | | H | -1.219019 | -2.701138 | 1.173573 | | H | -1.219204 | -2.700995 | -1.173623 | | H | -1.861729 | -1.052647 | -1.194191 | | H | 2.483241 | 0.363983 | 1.35301 | | H | 1.535833 | 1.629902 | 2.136026 | | H | 1.535454 | 1.630212 | -2.135954 | | H | 2.482999 | 0.364178 | -1.353294 | | H | 1.308788 | 2.844185 | 0.000143 | | H | 3.009896 | 2.355101 | -0.000045 | | B | -4.04504 | 1.927611 | -0.000238 | | O | -3.017507 | 1.286835 | 0.000325 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 Site 5 JP-10/BO** | | | | **vdW1 Site 6 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.162527 | 0.205488 | 0.426204 | | C | -0.368143 | -0.523045 | -0.860937 | | C | -1.13012 | 0.68876 | 1.106199 | | C | -1.894106 | -0.359941 | -0.748451 | | C | -2.11461 | -0.445938 | 0.772322 | | C | -1.708318 | 1.841577 | 0.263033 | | C | -2.235827 | 1.118831 | -1.014159 | | C | 0.974317 | -0.851769 | 1.196573 | | C | 0.162958 | -1.965522 | -0.768713 | | C | 1.407845 | -1.852431 | 0.119306 | | H | 0.815736 | 1.046829 | 0.169896 | | H | 0.008773 | -0.04685 | -1.775208 | | H | -1.010077 | 0.928408 | 2.168908 | | H | -2.46356 | -1.067913 | -1.361481 | | H | -1.838356 | -1.411742 | 1.205264 | | H | -3.145644 | -0.21559 | 1.065486 | | H | -0.950372 | 2.599159 | 0.039176 | | H | -2.524614 | 2.34076 | 0.796245 | | H | -3.317676 | 1.252281 | -1.121702 | | H | -1.767558 | 1.485479 | -1.933409 | | H | 0.340824 | -1.353571 | 1.939326 | | H | 1.81882 | -0.40456 | 1.729633 | | H | 0.370123 | -2.392356 | -1.755838 | | H | -0.58025 | -2.612251 | -0.285461 | | H | 2.237088 | -1.424372 | -0.454464 | | H | 1.73815 | -2.814426 | 0.526364 | | B | 4.557266 | 1.646835 | -0.392524 | | O | 3.492891 | 1.09006 | -0.242297 | |  |  |  |  | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.637852 | 0.879442 | -0.78586 | | C | 0.637917 | 0.87957 | 0.785708 | | C | 1.139585 | -0.533504 | -1.13123 | | C | 1.139677 | -0.533324 | 1.131267 | | C | 0.524162 | -1.376503 | 0.000113 | | C | 2.637908 | -0.60743 | -0.779722 | | C | 2.63797 | -0.607316 | 0.779648 | | C | -0.812056 | 1.194328 | -1.198756 | | C | -0.811956 | 1.194523 | 1.198678 | | C | -1.392267 | 1.954273 | -0.000074 | | H | 1.315775 | 1.643256 | -1.188833 | | H | 1.315882 | 1.643444 | 1.188495 | | H | 0.90332 | -0.849413 | -2.153785 | | H | 0.90349 | -0.849062 | 2.153892 | | H | -0.568595 | -1.389536 | 0.000163 | | H | 0.888195 | -2.411005 | 0.000181 | | H | 3.198459 | 0.231897 | -1.204337 | | H | 3.081648 | -1.52899 | -1.171585 | | H | 3.081734 | -1.528824 | 1.171607 | | H | 3.198565 | 0.232066 | 1.204094 | | H | -1.375171 | 0.265653 | -1.342777 | | H | -0.859089 | 1.758955 | -2.136174 | | H | -0.858909 | 1.759304 | 2.136007 | | H | -1.375067 | 0.265878 | 1.342897 | | H | -1.027715 | 2.989254 | -0.000177 | | H | -2.486951 | 1.984195 | -0.000031 | | B | -4.336727 | -1.72652 | -0.000581 | | O | -3.210586 | -1.281103 | 0.00058 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS1 JP-10/BO** | | | | **TS2 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.014145 | -0.652867 | 0.684473 | | C | 1.412093 | 0.825558 | 0.331264 | | C | -0.397908 | -0.788092 | 0.069935 | | C | 0.177615 | 1.347016 | -0.42613 | | C | -0.285182 | 0.092351 | -1.187829 | | C | -1.32501 | 0.059418 | 0.9287 | | C | -0.967 | 1.516019 | 0.595009 | | C | 2.099818 | -1.541239 | 0.046702 | | C | 2.709671 | 0.717782 | -0.490835 | | C | 3.321461 | -0.620345 | -0.058791 | | H | 0.986729 | -0.818203 | 1.76875 | | H | 1.59341 | 1.419609 | 1.235961 | | H | -0.724379 | -1.823657 | -0.075957 | | H | 0.367808 | 2.238616 | -1.033146 | | H | 0.443807 | -0.276043 | -1.914298 | | H | -1.242477 | 0.232569 | -1.702623 | | H | -1.404032 | -0.214336 | 1.984575 | | H | -2.517852 | -0.158877 | 0.496746 | | H | -1.818766 | 2.041493 | 0.143712 | | H | -0.663231 | 2.088068 | 1.477839 | | H | 1.789051 | -1.860625 | -0.955434 | | H | 2.286088 | -2.446937 | 0.632428 | | H | 3.373575 | 1.572145 | -0.325028 | | H | 2.479133 | 0.690212 | -1.562858 | | H | 3.790896 | -0.512868 | 0.926467 | | H | 4.084101 | -0.991898 | -0.750866 | | B | -3.871099 | -0.402171 | -0.015786 | | O | -5.003323 | -0.612752 | -0.402791 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.272786 | 0.43704 | -0.773867 | | C | 1.657749 | -0.134243 | -0.264942 | | C | -0.693408 | -0.527298 | -0.104895 | | C | 1.2437 | -1.321391 | 0.629803 | | C | -0.06892 | -0.804004 | 1.260335 | | C | -0.662033 | -1.890188 | -0.785316 | | C | 0.709879 | -2.45188 | -0.276863 | | C | 0.231941 | 1.90266 | -0.303205 | | C | 2.342391 | 1.042589 | 0.454247 | | C | 1.708923 | 2.292448 | -0.167823 | | H | 0.190162 | 0.385513 | -1.866026 | | H | 2.276986 | -0.475944 | -1.103781 | | H | -1.953494 | -0.0197 | -0.031817 | | H | 2.023053 | -1.640091 | 1.33136 | | H | 0.056591 | 0.082014 | 1.887152 | | H | -0.600989 | -1.573018 | 1.830007 | | H | -0.714841 | -1.810656 | -1.874767 | | H | -1.493793 | -2.520139 | -0.452655 | | H | 0.563981 | -3.372628 | 0.296965 | | H | 1.398352 | -2.677988 | -1.096942 | | H | -0.261933 | 1.977905 | 0.672902 | | H | -0.324796 | 2.540656 | -0.996547 | | H | 3.431321 | 1.008911 | 0.347088 | | H | 2.121365 | 1.010836 | 1.528122 | | H | 2.137468 | 2.470948 | -1.161349 | | H | 1.8629 | 3.19803 | 0.427544 | | B | -3.248166 | 0.498339 | 0.093944 | | O | -4.366196 | 0.956156 | 0.223522 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS3 JP-10/BO** | | | | **TS4 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.607771 | 0.923543 | -0.785755 | | C | 0.607835 | 0.923685 | 0.785556 | | C | 0.960913 | -0.531952 | -1.139281 | | C | 0.960789 | -0.531802 | 1.139312 | | C | 0.327335 | -1.322277 | 0.000038 | | C | 2.451824 | -0.753161 | -0.781217 | | C | 2.45174 | -0.753098 | 0.781417 | | C | -0.793095 | 1.408137 | -1.201704 | | C | -0.792854 | 1.408697 | 1.201659 | | C | -1.283753 | 2.22551 | -0.000164 | | H | 1.368206 | 1.605911 | -1.185579 | | H | 1.368468 | 1.605956 | 1.185159 | | H | 0.694378 | -0.832984 | -2.157382 | | H | 0.694161 | -0.832682 | 2.157432 | | H | -1.033643 | -1.319837 | -0.000488 | | H | 0.502984 | -2.403813 | 0.000131 | | H | 3.084718 | 0.031883 | -1.207289 | | H | 2.805394 | -1.711781 | -1.173338 | | H | 2.805291 | -1.711671 | 1.17367 | | H | 3.084573 | 0.032002 | 1.207475 | | H | -1.461472 | 0.555638 | -1.368372 | | H | -0.76841 | 1.980828 | -2.134342 | | H | -0.767684 | 1.982027 | 2.133898 | | H | -1.461329 | 0.556454 | 1.369348 | | H | -0.801824 | 3.210716 | -0.000412 | | H | -2.366632 | 2.385119 | -0.000092 | | B | -2.4122 | -1.581556 | -0.000581 | | O | -3.584652 | -1.90121 | 0.00049 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.213747 | 0.326327 | 0.446942 | | C | 0.580804 | 0.435358 | -0.878368 | | C | 0.388763 | -0.863395 | 1.18003 | | C | 1.615488 | -0.696317 | -0.7262 | | C | 1.876298 | -0.689633 | 0.792031 | | C | 0.041769 | -2.157509 | 0.415164 | | C | 0.875465 | -2.037511 | -0.896373 | | C | -0.231158 | 1.702107 | 1.100175 | | C | 1.110893 | 1.880914 | -0.888424 | | C | 0.081733 | 2.660094 | -0.058036 | | H | -1.443723 | 0.078661 | 0.157731 | | H | -0.058388 | 0.268589 | -1.757413 | | H | 0.16448 | -0.894361 | 2.251059 | | H | 2.494635 | -0.58278 | -1.369499 | | H | 2.321424 | 0.237993 | 1.164174 | | H | 2.493891 | -1.532413 | 1.123634 | | H | -1.031683 | -2.259664 | 0.231199 | | H | 0.352543 | -3.02936 | 0.999574 | | H | 1.588585 | -2.863416 | -0.983993 | | H | 0.251941 | -2.047171 | -1.795831 | | H | 0.556355 | 1.754419 | 1.86466 | | H | -1.181778 | 1.914116 | 1.603746 | | H | 1.231577 | 2.268912 | -1.904728 | | H | 2.092244 | 1.9255 | -0.400604 | | H | -0.823645 | 2.82898 | -0.653066 | | H | 0.44466 | 3.636396 | 0.277851 | | O | -3.997019 | -0.515425 | -0.371026 | | B | -2.846961 | -0.188723 | -0.152387 | |  |  |  |  | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS5 JP-10/BO** | | | | **TS6 JP-10/BO** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.152024 | -0.259404 | -0.170492 | | C | 0.812778 | 0.85797 | -0.716938 | | C | 0.771813 | -1.135205 | 0.692661 | | C | 2.165082 | 0.465655 | -0.095756 | | C | 1.739701 | -0.090964 | 1.275111 | | C | 1.702745 | -1.91494 | -0.255038 | | C | 2.663101 | -0.812678 | -0.796707 | | C | -1.23555 | 0.499338 | 0.583969 | | C | 0.227604 | 2.197526 | -0.225448 | | C | -1.262852 | 1.911628 | 0.025405 | | H | -0.599986 | -0.843706 | -0.986697 | | H | 0.8627 | 0.847086 | -1.81272 | | H | 0.238709 | -1.762772 | 1.415296 | | H | 2.895027 | 1.282631 | -0.08107 | | H | 1.255548 | 0.646406 | 1.923056 | | H | 2.571818 | -0.543889 | 1.825561 | | H | 1.144948 | -2.421675 | -1.048866 | | H | 2.256088 | -2.682014 | 0.296202 | | H | 3.70039 | -1.024896 | -0.518109 | | H | 2.630303 | -0.71854 | -1.886752 | | H | -1.190312 | 0.42443 | 1.674835 | | H | -2.364228 | -0.073817 | 0.30207 | | H | 0.386736 | 3.006316 | -0.945966 | | H | 0.7092 | 2.498045 | 0.712201 | | H | -1.804703 | 1.919939 | -0.929448 | | H | -1.744205 | 2.63561 | 0.689125 | | O | -4.680504 | -1.251177 | -0.275972 | | B | -3.619678 | -0.698657 | -0.06431 | | | | | |  |  |  |  | | --- | --- | --- | --- | | O | 4.426367 | -1.442731 | 0.000026 | | C | -0.127232 | -0.092518 | -0.786394 | | C | -0.127238 | -0.092561 | 0.786382 | | C | -1.619648 | 0.053471 | -1.131741 | | C | -1.619654 | 0.053449 | 1.131734 | | C | -2.119705 | 0.968621 | 0.000005 | | C | -2.322109 | -1.271409 | -0.779523 | | C | -2.32216 | -1.2714 | 0.779494 | | C | 0.767042 | 1.087868 | -1.214427 | | C | 0.767054 | 1.087789 | 1.214479 | | C | 1.628388 | 1.368854 | 0.00003 | | H | 0.278234 | -1.029132 | -1.188688 | | H | 0.278203 | -1.029204 | 1.18863 | | H | -1.804179 | 0.400179 | -2.154554 | | H | -1.804175 | 0.400144 | 2.154554 | | H | -1.663917 | 1.963818 | 0.000015 | | H | -3.209013 | 1.087544 | 0.000006 | | H | -1.800546 | -2.134681 | -1.204705 | | H | -3.34413 | -1.280895 | -1.172019 | | H | -3.344215 | -1.280803 | 1.171914 | | H | -1.800692 | -2.134704 | 1.204731 | | H | 0.158079 | 1.974289 | -1.442602 | | H | 1.351638 | 0.864823 | -2.113895 | | H | 1.351648 | 0.864692 | 2.113936 | | H | 0.158095 | 1.9742 | 1.442706 | | H | 2.236527 | 2.277895 | 0.000061 | | B | 3.522055 | -0.631545 | -0.000096 | | H | 2.508793 | 0.428426 | -0.000059 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 HBO/R1** | | | | **vdW2 HBO/R2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.06015 | -0.422629 | 0.874749 | | C | 1.683835 | 0.746792 | 0.030983 | | C | -0.447076 | -0.34187 | 0.505197 | | C | 0.47096 | 1.331998 | -0.719007 | | C | -0.375063 | 0.072691 | -0.979292 | | C | -0.961317 | 0.928626 | 1.122785 | | C | -0.411005 | 2.076819 | 0.307074 | | C | 1.794445 | -1.701016 | 0.426944 | | C | 2.758687 | 0.087681 | -0.853518 | | C | 3.142105 | -1.191146 | -0.098638 | | H | 1.203123 | -0.265511 | 1.950526 | | H | 2.14507 | 1.50528 | 0.676069 | | H | -1.008942 | -1.251622 | 0.74221 | | H | 0.736193 | 1.925971 | -1.600145 | | H | 0.117556 | -0.665117 | -1.618125 | | H | -1.357337 | 0.302588 | -1.405502 | | H | -1.238685 | 1.012076 | 2.170177 | | H | -3.460249 | 0.091031 | 0.410367 | | H | -1.20955 | 2.639341 | -0.199864 | | H | 0.156621 | 2.801451 | 0.904573 | | H | 1.242945 | -2.194333 | -0.382556 | | H | 1.891883 | -2.425714 | 1.24156 | | H | 3.607766 | 0.754251 | -1.035732 | | H | 2.336615 | -0.173242 | -1.83184 | | H | 3.797298 | -0.941438 | 0.744653 | | H | 3.668159 | -1.921403 | -0.722332 | | O | -5.36655 | -1.047284 | -0.458145 | | B | -4.398078 | -0.468602 | -0.016509 | | | | | |  |  |  |  | | --- | --- | --- | --- | | O | 5.123371 | 0.217198 | 0.069428 | | C | -0.064226 | -0.294278 | -0.661145 | | C | -1.607255 | -0.560083 | -0.393209 | | C | 0.120752 | 1.001773 | 0.098204 | | C | -2.01886 | 0.628464 | 0.502696 | | C | -0.736988 | 0.852064 | 1.345055 | | C | -0.504482 | 2.174161 | -0.632254 | | C | -2.030907 | 1.910148 | -0.360746 | | C | 0.662111 | -1.543373 | -0.127899 | | C | -1.672044 | -1.950518 | 0.263717 | | C | -0.392275 | -2.654465 | -0.201505 | | H | 0.137807 | -0.164145 | -1.730847 | | H | -2.176664 | -0.558352 | -1.331137 | | H | -2.945215 | 0.458197 | 1.063345 | | H | -0.473669 | 0.00559 | 1.983041 | | H | -0.783447 | 1.760263 | 1.954103 | | H | -0.258675 | 2.183856 | -1.69766 | | H | -0.19172 | 3.131172 | -0.203107 | | H | -2.478231 | 2.744478 | 0.189121 | | H | -2.602531 | 1.777103 | -1.284574 | | H | 0.968324 | -1.390562 | 0.913524 | | H | 1.565789 | -1.768771 | -0.702901 | | H | -2.585908 | -2.488655 | -0.008163 | | H | -1.665447 | -1.854239 | 1.356303 | | H | -0.508084 | -2.986775 | -1.2402 | | H | -0.137093 | -3.532153 | 0.401065 | | B | 3.957036 | 0.541682 | 0.122606 | | H | 2.827653 | 0.853644 | 0.172148 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 HBO/R3** | | | | **vdW2 HBO/R4** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | O | 4.86964 | -1.191161 | 0.000139 | | C | -0.916675 | 0.832268 | 0.786703 | | C | -0.916611 | 0.83217 | -0.786787 | | C | -1.132834 | -0.653066 | 1.137569 | | C | -1.132695 | -0.653216 | -1.137485 | | C | -0.410766 | -1.33718 | 0.000132 | | C | -2.59959 | -1.013041 | 0.780758 | | C | -2.59949 | -1.013165 | -0.780807 | | C | 0.450905 | 1.407005 | 1.19697 | | C | 0.450982 | 1.406901 | -1.197024 | | C | 0.879488 | 2.262628 | -0.00005 | | H | -1.726187 | 1.451752 | 1.192834 | | H | -1.726112 | 1.451575 | -1.193061 | | H | -0.838361 | -0.924515 | 2.155738 | | H | -0.838096 | -0.924792 | -2.155583 | | H | -0.146682 | -2.393335 | 0.00022 | | H | -3.304847 | -0.291973 | 1.207396 | | H | -2.859906 | -2.00122 | 1.172397 | | H | -2.859732 | -2.001413 | -1.172321 | | H | -3.304709 | -0.292181 | -1.207651 | | H | 1.165834 | 0.586874 | 1.336487 | | H | 0.402615 | 1.963669 | 2.138547 | | H | 0.402733 | 1.963488 | -2.138649 | | H | 1.165933 | 0.586773 | -1.336439 | | H | 0.324739 | 3.208829 | -0.000109 | | H | 1.947456 | 2.504643 | -0.000027 | | B | 3.661678 | -1.282694 | -0.00009 | | H | 2.493526 | -1.373227 | -0.000319 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.055228 | 0.229493 | 0.623954 | | C | 0.392086 | 0.438239 | -0.851985 | | C | 1.159863 | -0.613511 | 1.202806 | | C | 1.756555 | -0.273995 | -0.966436 | | C | 2.368497 | -0.027724 | 0.426916 | | C | 1.073264 | -2.026124 | 0.579827 | | C | 1.48999 | -1.791639 | -0.904436 | | C | -0.458308 | 1.51323 | 1.224355 | | C | 0.349647 | 1.969673 | -1.00975 | | C | -0.726992 | 2.405464 | -0.003088 | | H | -2.359343 | -0.675068 | 0.235686 | | H | -0.342831 | -0.017667 | -1.534108 | | H | 1.230797 | -0.601632 | 2.294703 | | H | 2.359935 | 0.041573 | -1.824303 | | H | 2.5543 | 1.027321 | 0.651442 | | H | 3.294455 | -0.591683 | 0.591728 | | H | 0.070275 | -2.450357 | 0.677825 | | H | 1.76995 | -2.704924 | 1.082837 | | H | 2.398757 | -2.351273 | -1.148827 | | H | 0.716051 | -2.098886 | -1.614862 | | H | 0.318075 | 1.962923 | 1.864127 | | H | -1.340777 | 1.375557 | 1.861634 | | H | 0.13442 | 2.282177 | -2.036644 | | H | 1.317503 | 2.401432 | -0.727178 | | H | -1.720778 | 2.187241 | -0.411151 | | H | -0.694247 | 3.474361 | 0.228918 | | O | -4.634075 | -1.193439 | -0.260676 | | B | -3.478583 | -0.930444 | -0.007882 | |  |  |  |  | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 HBO/R5** | | | | **vdW2 HBO/R6** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | O | -5.066482 | -1.266714 | -0.438997 | | C | -0.034586 | -0.172982 | 0.443366 | | C | 0.509464 | 0.483381 | -0.875785 | | C | 1.244805 | -0.717143 | 1.124697 | | C | 2.017515 | 0.184796 | -0.801045 | | C | 2.291679 | 0.326607 | 0.707343 | | C | 1.708459 | -1.948575 | 0.325934 | | C | 2.225711 | -1.328174 | -1.007438 | | C | -0.740083 | 0.938098 | 1.15163 | | C | 0.158132 | 1.986007 | -0.793714 | | C | -0.971499 | 2.10785 | 0.247828 | | H | -0.718435 | -1.01278 | 0.233852 | | H | 0.059486 | 0.032983 | -1.769112 | | H | 1.131223 | -0.890707 | 2.199964 | | H | 2.621625 | 0.81316 | -1.464983 | | H | 2.087644 | 1.324569 | 1.106742 | | H | 3.312916 | 0.03832 | 0.981279 | | H | 0.898477 | -2.669341 | 0.173873 | | H | 2.513533 | -2.468514 | 0.855524 | | H | 3.286041 | -1.554008 | -1.160518 | | H | 1.683695 | -1.695621 | -1.884826 | | H | -1.177651 | 0.83472 | 2.140656 | | H | -3.150043 | -0.200397 | 0.492309 | | H | 1.031857 | 2.552422 | -0.454529 | | H | -1.952938 | 2.035556 | -0.251179 | | H | -0.966122 | 3.0691 | 0.773844 | | B | -4.092356 | -0.72466 | 0.034675 | | H | -0.125254 | 2.388358 | -1.771188 | | | | | |  |  |  |  | | --- | --- | --- | --- | | O | 3.113165 | 1.684621 | -0.057578 | | C | 0.065817 | 0.388285 | 0.594482 | | C | -0.062709 | -0.295893 | -0.816015 | | C | -1.384372 | 0.384472 | 1.109777 | | C | -1.570006 | -0.588815 | -0.921993 | | C | -1.922005 | -0.937643 | 0.535148 | | C | -2.186724 | 1.418037 | 0.298252 | | C | -2.311302 | 0.748678 | -1.103608 | | C | 1.047508 | -0.471802 | 1.420263 | | C | 0.832324 | -1.555289 | -0.784347 | | C | 1.683813 | -1.401938 | 0.436901 | | H | 0.453939 | 1.408295 | 0.509897 | | H | 0.260856 | 0.377793 | -1.61905 | | H | -1.464272 | 0.510115 | 2.195273 | | H | -1.819224 | -1.343749 | -1.676288 | | H | -1.402322 | -1.824194 | 0.913634 | | H | -2.998368 | -1.069053 | 0.694926 | | H | -1.680481 | 2.387816 | 0.262962 | | H | -3.173399 | 1.57874 | 0.745387 | | H | -3.360503 | 0.575163 | -1.364915 | | H | -1.870699 | 1.352566 | -1.903462 | | H | 0.504657 | -1.038368 | 2.196117 | | H | 1.780423 | 0.148164 | 1.949135 | | H | 1.416517 | -1.672533 | -1.706469 | | H | 0.209439 | -2.463398 | -0.713237 | | H | 2.447486 | -2.124095 | 0.716566 | | B | 3.387029 | 0.741116 | -0.769686 | | H | 3.701412 | -0.114369 | -1.50458 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW1 JP-10/BO2** | | | | **vdW2 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -1.733966 | -0.657576 | -0.622443 | | C | -1.572927 | 0.888352 | -0.38956 | | C | -0.356978 | -1.214031 | -0.220451 | | C | -0.121189 | 1.013045 | 0.10502 | | C | 0.049713 | -0.275864 | 0.929334 | | C | 0.662361 | -0.80827 | -1.301609 | | C | 0.807975 | 0.730204 | -1.092168 | | C | -2.915717 | -1.088308 | 0.266403 | | C | -2.665862 | 1.270216 | 0.625946 | | C | -3.740746 | 0.191289 | 0.447992 | | H | -1.955502 | -0.886144 | -1.672926 | | H | -1.717476 | 1.453584 | -1.319335 | | H | -0.359232 | -2.285425 | 0.008786 | | H | 0.090196 | 1.954859 | 0.624349 | | H | -0.608634 | -0.332159 | 1.801124 | | H | 1.080443 | -0.4452 | 1.257632 | | H | 0.318897 | -1.068645 | -2.308095 | | H | 1.61446 | -1.320514 | -1.13157 | | H | 1.841191 | 1.006651 | -0.85549 | | H | 0.516654 | 1.307739 | -1.975694 | | H | -2.548847 | -1.432592 | 1.241258 | | H | -3.484595 | -1.913231 | -0.174819 | | H | -3.039899 | 2.286842 | 0.466268 | | H | -2.266129 | 1.228213 | 1.646627 | | H | -4.319547 | 0.391585 | -0.461991 | | H | -4.445422 | 0.13849 | 1.284627 | | O | 3.763701 | -1.111134 | 0.865873 | | B | 4.21371 | -0.058002 | 0.447736 | | O | 4.703664 | 1.100087 | -0.0109 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.16166 | 0.488401 | -0.225288 | | C | 1.61713 | 0.09062 | -0.665799 | | C | -0.287904 | -0.727438 | 0.605263 | | C | 1.805067 | -1.299511 | -0.033957 | | C | 1.024377 | -1.159991 | 1.283854 | | C | -0.527164 | -1.904632 | -0.360868 | | C | 0.916766 | -2.298162 | -0.800377 | | C | 0.305033 | 1.81454 | 0.543347 | | C | 2.529535 | 1.206896 | -0.124616 | | C | 1.604452 | 2.423289 | 0.002806 | | H | -0.491735 | 0.637905 | -1.093349 | | H | 1.704589 | 0.036342 | -1.758443 | | H | -1.118391 | -0.526642 | 1.29461 | | H | 2.852316 | -1.609528 | 0.055029 | | H | 1.434645 | -0.410192 | 1.966064 | | H | 0.92807 | -2.108407 | 1.824637 | | H | -1.158864 | -1.6201 | -1.209037 | | H | -1.023697 | -2.734528 | 0.152676 | | H | 1.148209 | -3.326944 | -0.5052 | | H | 1.063894 | -2.226617 | -1.882719 | | H | 0.407146 | 1.621636 | 1.618858 | | H | -0.568769 | 2.458919 | 0.406117 | | H | 3.393284 | 1.383558 | -0.773895 | | H | 2.91791 | 0.932764 | 0.864127 | | H | 1.424185 | 2.857821 | -0.987865 | | H | 2.012192 | 3.212981 | 0.642482 | | O | -3.517514 | -0.662742 | 0.521782 | | B | -3.30461 | 0.494362 | -0.113511 | | O | -3.144441 | 1.555885 | -0.695874 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW3 JP-10/BO2** | | | | **vdW4 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -1.848 | -0.062721 | -0.280286 | | C | -0.950366 | -0.22457 | 0.999284 | | C | -1.119511 | 1.031777 | -1.079208 | | C | 0.176726 | 0.795086 | 0.761763 | | C | 0.356206 | 0.722168 | -0.767665 | | C | -1.306264 | 2.371276 | -0.342078 | | C | -0.409167 | 2.210726 | 0.9226 | | C | -1.890031 | -1.456714 | -0.933685 | | C | -0.523211 | -1.704702 | 1.022775 | | C | -1.614743 | -2.425451 | 0.222509 | | H | -2.865102 | 0.258149 | -0.021267 | | H | -1.505228 | 0.018856 | 1.914346 | | H | -1.389488 | 1.061417 | -2.140692 | | H | 1.065389 | 0.617618 | 1.378821 | | H | 0.676365 | -0.257269 | -1.135205 | | H | 1.034818 | 1.490442 | -1.158953 | | H | -2.356818 | 2.55661 | -0.096523 | | H | -0.962861 | 3.205303 | -0.963089 | | H | 0.389595 | 2.959844 | 0.934849 | | H | -0.969154 | 2.313094 | 1.857577 | | H | -1.09728 | -1.547386 | -1.686561 | | H | -2.841563 | -1.644706 | -1.441659 | | H | -0.413402 | -2.084165 | 2.043971 | | H | 0.445349 | -1.833515 | 0.525064 | | H | -2.516435 | -2.534639 | 0.837519 | | H | -1.316364 | -3.424513 | -0.111398 | | O | 3.156471 | -1.643754 | -0.445984 | | B | 3.285811 | -0.455079 | -0.195834 | | O | 3.46394 | 0.84113 | 0.081774 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.15811 | 0.268219 | 0.783547 | | C | 0.165566 | 0.382358 | -0.785028 | | C | 1.571567 | -0.250323 | 1.101434 | | C | 1.581782 | -0.089987 | -1.156651 | | C | 2.41678 | 0.444834 | 0.019701 | | C | 1.65339 | -1.7195 | 0.645209 | | C | 1.655182 | -1.609471 | -0.910213 | | C | -0.180507 | 1.679169 | 1.300142 | | C | -0.161088 | 1.855534 | -1.09302 | | C | -0.934201 | 2.339986 | 0.139337 | | H | -0.590145 | -0.448811 | 1.151319 | | H | -0.58526 | -0.265417 | -1.255247 | | H | 1.87911 | -0.084191 | 2.139839 | | H | 1.901164 | 0.218486 | -2.158299 | | H | 2.425625 | 1.535854 | 0.097041 | | H | 3.453483 | 0.089661 | 0.000418 | | H | 0.816974 | -2.313907 | 1.026711 | | H | 2.576765 | -2.183949 | 1.006883 | | H | 2.57572 | -2.025727 | -1.332605 | | H | 0.814828 | -2.138035 | -1.371825 | | H | 0.743523 | 2.233067 | 1.507398 | | H | -0.75556 | 1.649868 | 2.231423 | | H | -0.724208 | 1.963283 | -2.025526 | | H | 0.765522 | 2.43249 | -1.202677 | | H | -1.963399 | 1.966205 | 0.099447 | | H | -0.978196 | 3.431094 | 0.220026 | | O | -3.608864 | -0.278832 | -0.369134 | | B | -2.87082 | -1.190403 | -0.029947 | | O | -2.086302 | -2.210278 | 0.337718 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW5 JP-10/BO2** | | | | **vdW6 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.403328 | 0.446756 | 0.709745 | | C | 0.521435 | 0.320123 | -0.851471 | | C | 0.628772 | -1.000127 | 1.193848 | | C | 0.775776 | -1.187054 | -1.050657 | | C | 1.634975 | -1.555126 | 0.17028 | | C | -0.626421 | -1.815944 | 0.829046 | | C | -0.534373 | -1.931596 | -0.724021 | | C | 1.465413 | 1.479047 | 1.139874 | | C | 1.678953 | 1.253968 | -1.267317 | | C | 2.493992 | 1.557888 | 0.000803 | | H | -0.590268 | 0.78773 | 1.035101 | | H | -0.40059 | 0.609864 | -1.368139 | | H | 0.914753 | -1.071191 | 2.249182 | | H | 1.192741 | -1.434454 | -2.033104 | | H | 2.61406 | -1.074466 | 0.193819 | | H | 1.777241 | -2.637579 | 0.272452 | | H | -1.545006 | -1.329964 | 1.175753 | | H | -0.592346 | -2.80425 | 1.299583 | | H | -0.469013 | -2.979685 | -1.034255 | | H | -1.39195 | -1.490182 | -1.240336 | | H | 1.915997 | 1.224827 | 2.105971 | | H | 0.98355 | 2.456655 | 1.258657 | | H | 1.259603 | 2.18722 | -1.660522 | | H | 2.287329 | 0.816406 | -2.066956 | | H | 2.974819 | 2.540358 | -0.047577 | | H | 3.29245 | 0.825396 | 0.141918 | | O | -3.063842 | 0.977132 | 1.230449 | | B | -3.080373 | 0.84876 | -0.099884 | | O | -3.120234 | 0.738106 | -1.315814 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.977908 | -0.877496 | -0.785649 | | C | -0.977702 | -0.87734 | 0.785796 | | C | -1.606552 | 0.483743 | -1.131251 | | C | -1.606257 | 0.483964 | 1.131272 | | C | -1.071808 | 1.38053 | -0.000147 | | C | -3.105186 | 0.418825 | -0.779469 | | C | -3.104983 | 0.418927 | 0.779897 | | C | 0.494623 | -1.056724 | -1.199686 | | C | 0.49493 | -1.056482 | 1.19949 | | C | 1.14034 | -1.761253 | -0.000111 | | H | -1.581585 | -1.700803 | -1.189035 | | H | -1.581271 | -1.700569 | 1.189506 | | H | -1.40071 | 0.819608 | -2.153928 | | H | -1.40018 | 0.820038 | 2.153832 | | H | 0.01465 | 1.501226 | -0.000314 | | H | -1.531306 | 2.375952 | -0.000191 | | H | -3.586269 | -0.468416 | -1.204047 | | H | -3.631519 | 1.295575 | -1.171439 | | H | -3.631241 | 1.295708 | 1.171895 | | H | -3.585915 | -0.468278 | 1.204724 | | H | 0.961262 | -0.075996 | -1.346622 | | H | 0.594282 | -1.614165 | -2.137056 | | H | 0.594819 | -1.613738 | 2.136944 | | H | 0.961606 | -0.075725 | 1.346123 | | H | 0.86373 | -2.822782 | 0.000032 | | H | 2.235396 | -1.711873 | -0.000259 | | O | 2.706157 | 1.68228 | -0.00058 | | B | 3.6617 | 0.923826 | -0.000087 | | O | 4.708689 | 0.090837 | 0.000506 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS1 JP-10/BO2** | | | | **TS2 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.461748 | -0.733085 | 0.563655 | | C | 1.555716 | 0.832737 | 0.479819 | | C | 0.098788 | -1.036427 | -0.092018 | | C | 0.228045 | 1.222832 | -0.192899 | | C | 0.008014 | 0.055638 | -1.17138 | | C | -0.983926 | -0.565673 | 0.886173 | | C | -0.906085 | 0.98041 | 0.824477 | | C | 2.691874 | -1.265256 | -0.196379 | | C | 2.833431 | 1.126826 | -0.327854 | | C | 3.705664 | -0.117218 | -0.121321 | | H | 1.484092 | -1.086159 | 1.602393 | | H | 1.634354 | 1.285308 | 1.476397 | | H | -0.016876 | -2.072452 | -0.42654 | | H | 0.224305 | 2.227651 | -0.628425 | | H | 0.77758 | -0.025058 | -1.943699 | | H | -0.971197 | 0.08674 | -1.662039 | | H | -0.896129 | -0.990443 | 1.891441 | | H | -1.981254 | -0.952422 | 0.50525 | | H | -1.843886 | 1.425754 | 0.474011 | | H | -0.688094 | 1.421461 | 1.802388 | | H | 2.433546 | -1.462564 | -1.243937 | | H | 3.063523 | -2.203324 | 0.227974 | | H | 3.317527 | 2.054874 | -0.007511 | | H | 2.593016 | 1.23759 | -1.392298 | | H | 4.161169 | -0.089399 | 0.875909 | | H | 4.514842 | -0.20632 | -0.853454 | | O | -3.405046 | -1.363598 | -0.178396 | | B | -3.91876 | -0.137198 | -0.216502 | | O | -4.391497 | 0.992354 | -0.262727 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.093937 | 0.463436 | -0.416197 | | C | 1.637901 | 0.196117 | -0.587296 | | C | -0.34347 | -0.772204 | 0.37499 | | C | 1.846976 | -1.148913 | 0.133745 | | C | 0.848113 | -1.044085 | 1.30439 | | C | -0.333849 | -1.999313 | -0.543368 | | C | 1.197012 | -2.259471 | -0.716601 | | C | -0.018912 | 1.816779 | 0.30928 | | C | 2.334867 | 1.413904 | 0.047065 | | C | 1.292152 | 2.534703 | -0.033508 | | H | -0.42108 | 0.512641 | -1.382413 | | H | 1.91195 | 0.116686 | -1.646604 | | H | -1.328697 | -0.641096 | 0.944487 | | H | 2.888452 | -1.347819 | 0.409848 | | H | 1.061077 | -0.231058 | 2.002122 | | H | 0.744556 | -1.978725 | 1.864942 | | H | -0.845391 | -1.804541 | -1.490463 | | H | -0.828408 | -2.849203 | -0.063256 | | H | 1.467796 | -3.248704 | -0.334118 | | H | 1.515624 | -2.211219 | -1.762296 | | H | -0.089074 | 1.665696 | 1.393678 | | H | -0.909247 | 2.370339 | -0.003625 | | H | 3.274313 | 1.656983 | -0.459686 | | H | 2.576923 | 1.207752 | 1.096903 | | H | 1.242573 | 2.922926 | -1.057762 | | H | 1.509437 | 3.377218 | 0.630821 | | O | -2.849437 | -0.34976 | 1.145073 | | B | -3.10113 | 0.267469 | -0.00844 | | O | -3.349753 | 0.842143 | -1.061996 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS3 JP-10/BO2** | | | | **TS4 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 1.473689 | 0.172466 | -0.778193 | | C | 1.457155 | 0.171799 | 0.79412 | | C | 0.473715 | -0.937825 | -1.14212 | | C | 0.449386 | -0.938525 | 1.135946 | | C | -0.557811 | -0.832391 | -0.013905 | | C | 1.110152 | -2.297323 | -0.777012 | | C | 1.093347 | -2.297867 | 0.783749 | | C | 1.076681 | 1.60135 | -1.195021 | | C | 1.051985 | 1.60047 | 1.203803 | | C | 1.469445 | 2.466121 | 0.008875 | | H | 2.470235 | -0.067359 | -1.169414 | | H | 2.44517 | -0.068761 | 1.205979 | | H | 0.084412 | -0.88238 | -2.163557 | | H | 0.038501 | -0.883692 | 2.148941 | | H | -1.097534 | 0.184839 | -0.020238 | | H | -1.335245 | -1.604329 | -0.022433 | | H | 2.118605 | -2.387753 | -1.192168 | | H | 0.51353 | -3.123611 | -1.176067 | | H | 0.48813 | -3.124326 | 1.169276 | | H | 2.092612 | -2.38877 | 1.220449 | | H | -0.005082 | 1.666778 | -1.35561 | | H | 1.563873 | 1.905712 | -2.126946 | | H | 1.520056 | 1.904021 | 2.145738 | | H | -0.032795 | 1.66596 | 1.342189 | | H | 2.555698 | 2.618377 | 0.020085 | | H | 0.994522 | 3.452237 | 0.004353 | | O | -2.249682 | 1.193759 | -0.026215 | | B | -3.313376 | 0.391132 | -0.006537 | | O | -4.304602 | -0.327792 | 0.011297 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.444979 | 0.324198 | -0.691828 | | C | -0.423126 | 0.276705 | 0.843049 | | C | -0.807513 | -1.062977 | -1.174787 | | C | -0.888796 | -1.169455 | 1.103095 | | C | -1.85288 | -1.408409 | -0.07393 | | C | 0.325257 | -2.047677 | -0.814709 | | C | 0.282278 | -2.105768 | 0.742359 | | C | -1.15478 | 1.589083 | -1.14743 | | C | -1.352682 | 1.438944 | 1.245858 | | C | -1.170699 | 2.461615 | 0.115002 | | H | 0.824718 | 0.52662 | -1.135105 | | H | 0.57703 | 0.44793 | 1.264183 | | H | -1.148107 | -1.104823 | -2.212929 | | H | -1.2994 | -1.32494 | 2.105511 | | H | -2.729179 | -0.752984 | -0.077701 | | H | -2.189747 | -2.447031 | -0.160914 | | H | 1.288063 | -1.716321 | -1.208457 | | H | 0.105127 | -3.024928 | -1.254782 | | H | 0.079486 | -3.123646 | 1.08929 | | H | 1.218519 | -1.776324 | 1.199953 | | H | -2.176208 | 1.298894 | -1.437058 | | H | -0.691871 | 2.054015 | -2.022654 | | H | -1.096634 | 1.834191 | 2.232388 | | H | -2.395012 | 1.099058 | 1.280766 | | H | -0.205829 | 2.968082 | 0.22338 | | H | -1.951887 | 3.226575 | 0.090591 | | O | 2.366794 | 0.724818 | -1.26286 | | B | 2.706408 | 0.570636 | -0.020667 | | O | 3.031508 | 0.423293 | 1.168709 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **TS5 JP-10/BO2** | | | | **TS6 JP-10/BO2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.071036 | -0.107928 | 0.655572 | | C | 0.261834 | 0.019994 | -0.896666 | | C | 1.513979 | 0.022421 | 1.198059 | | C | 1.792314 | 0.100544 | -1.04137 | | C | 2.197153 | 0.948066 | 0.175925 | | C | 2.225348 | -1.309672 | 0.892464 | | C | 2.378046 | -1.274084 | -0.658891 | | C | -0.884744 | 1.019391 | 1.052585 | | C | -0.504735 | 1.295287 | -1.321317 | | C | -0.825955 | 2.085851 | -0.039957 | | H | -0.335412 | -1.086188 | 0.939478 | | H | -0.129378 | -0.856396 | -1.425102 | | H | 1.567087 | 0.32727 | 2.2491 | | H | 2.12024 | 0.466932 | -2.02035 | | H | 1.813721 | 1.969845 | 0.157613 | | H | 3.283362 | 0.989451 | 0.318598 | | H | 1.653634 | -2.173771 | 1.244574 | | H | 3.20367 | -1.339798 | 1.383573 | | H | 3.430288 | -1.341325 | -0.953525 | | H | 1.84535 | -2.092073 | -1.153734 | | H | -0.745007 | 1.390622 | 2.074571 | | H | -1.949186 | 0.614591 | 1.05655 | | H | -1.439347 | 1.011728 | -1.81748 | | H | 0.068411 | 1.888561 | -2.042428 | | H | -1.764468 | 2.642756 | -0.118957 | | H | -0.042865 | 2.814593 | 0.188559 | | O | -3.374455 | 0.075284 | 0.461825 | | B | -2.931365 | -1.08289 | -0.021543 | | O | -2.534162 | -2.151732 | -0.470794 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.6221 | 0.242391 | 1.145214 | | C | -1.25705 | 1.230288 | 0.103144 | | C | -0.687303 | -1.120015 | 0.416646 | | C | -1.758148 | 0.281997 | -0.998177 | | C | -0.609625 | -0.735331 | -1.073157 | | C | -2.149219 | -1.594084 | 0.502559 | | C | -2.898026 | -0.576003 | -0.41127 | | C | 0.784274 | 0.777413 | 1.46071 | | C | -0.122676 | 2.179396 | -0.350183 | | C | 1.14675 | 1.711751 | 0.335072 | | H | -1.210665 | 0.194428 | 2.068531 | | H | -2.082584 | 1.810211 | 0.532439 | | H | 0.052474 | -1.845506 | 0.767664 | | H | -2.019477 | 0.794391 | -1.930776 | | H | 0.344775 | -0.31488 | -1.392966 | | H | -0.838284 | -1.58361 | -1.727985 | | H | -2.525305 | -1.602268 | 1.530477 | | H | -2.241004 | -2.612413 | 0.111697 | | H | -3.445207 | -1.086609 | -1.209635 | | H | -3.620937 | 0.035073 | 0.139524 | | H | 1.521281 | -0.015226 | 1.634808 | | H | 0.763467 | 1.384754 | 2.379045 | | H | -0.313603 | 3.210254 | -0.019625 | | H | -0.023479 | 2.223581 | -1.440695 | | H | 1.945434 | 2.439927 | 0.504286 | | H | 1.8313 | 0.984422 | -0.587957 | | O | 2.848651 | 0.031577 | -1.288445 | | B | 2.90094 | -0.895152 | -0.369275 | | O | 2.95083 | -1.772526 | 0.501469 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 BO2/R1** | | | | **vdW2 BO2/R2** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -1.145326 | -0.498976 | -0.822161 | | C | -1.910508 | 0.708415 | -0.172209 | | C | 0.312293 | -0.294249 | -0.318987 | | C | -0.808716 | 1.443633 | 0.614952 | | C | 0.072618 | 0.276784 | 1.094174 | | C | 0.810904 | 0.930558 | -1.03766 | | C | 0.128733 | 2.12542 | -0.405965 | | C | -1.848343 | -1.77 | -0.307723 | | C | -3.028493 | 0.076062 | 0.677497 | | C | -3.266313 | -1.295353 | 0.033339 | | H | -1.186787 | -0.464961 | -1.917362 | | H | -2.347663 | 1.364228 | -0.935655 | | H | 0.934914 | -1.191428 | -0.400543 | | H | -1.185965 | 2.115398 | 1.392873 | | H | -0.440962 | -0.419185 | 1.761751 | | H | 0.994247 | 0.609259 | 1.582448 | | H | 1.12013 | 0.908097 | -2.081592 | | H | 2.666387 | 0.866524 | -0.243965 | | H | 0.845959 | 2.784929 | 0.105531 | | H | -0.407131 | 2.745804 | -1.134512 | | H | -1.35236 | -2.141163 | 0.596925 | | H | -1.824641 | -2.578269 | -1.045094 | | H | -3.925784 | 0.702188 | 0.707892 | | H | -2.690223 | -0.055176 | 1.712581 | | H | -3.848863 | -1.176514 | -0.888106 | | H | -3.809671 | -1.990034 | 0.681948 | | O | 3.49541 | 0.65503 | 0.227456 | | B | 3.834296 | -0.626647 | 0.179462 | | O | 4.177821 | -1.800058 | 0.157047 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.065223 | 0.365085 | -0.467204 | | C | 1.640829 | 0.569357 | -0.542133 | | C | 0.021697 | -0.955831 | 0.269699 | | C | 2.198373 | -0.665873 | 0.199181 | | C | 1.131769 | -0.883022 | 1.303993 | | C | 0.410667 | -2.121412 | -0.617461 | | C | 1.968788 | -1.913939 | -0.683122 | | C | -0.477271 | 1.613032 | 0.255581 | | C | 1.902739 | 1.929127 | 0.129131 | | C | 0.580385 | 2.690098 | -0.014491 | | H | -0.378273 | 0.281381 | -1.465938 | | H | 1.982679 | 0.587437 | -1.584285 | | H | -1.878316 | -1.120725 | 0.86894 | | H | 3.231623 | -0.545001 | 0.543495 | | H | 1.047619 | -0.052722 | 2.007636 | | H | 1.277298 | -1.81586 | 1.856936 | | H | -0.068066 | -2.078157 | -1.599034 | | H | 0.163848 | -3.083545 | -0.158218 | | H | 2.491572 | -2.783002 | -0.271724 | | H | 2.324172 | -1.764345 | -1.707027 | | H | -0.555024 | 1.428744 | 1.333838 | | H | -1.472768 | 1.886663 | -0.10483 | | H | 2.753885 | 2.447837 | -0.323666 | | H | 2.136453 | 1.788506 | 1.191489 | | H | 0.473639 | 3.06144 | -1.040555 | | H | 0.500106 | 3.549174 | 0.658941 | | O | -2.851599 | -1.038372 | 0.927254 | | B | -3.369869 | -0.240397 | 0.004668 | | O | -3.878438 | 0.495175 | -0.830801 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 BO2/R3** | | | | **vdW2 BO2/R4** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | -0.881412 | 0.968179 | 0.764356 | | C | -0.896361 | 0.922574 | -0.807796 | | C | -1.378623 | -0.434644 | 1.163495 | | C | -1.399997 | -0.501022 | -1.115107 | | C | -0.830794 | -1.288451 | 0.043029 | | C | -2.890684 | -0.517608 | 0.821181 | | C | -2.905293 | -0.563273 | -0.740169 | | C | 0.573829 | 1.281861 | 1.15609 | | C | 0.5513 | 1.212325 | -1.244838 | | C | 1.167502 | 1.982667 | -0.071123 | | H | -1.554321 | 1.741944 | 1.153641 | | H | -1.577253 | 1.672583 | -1.228412 | | H | -1.132528 | -0.73177 | 2.186977 | | H | -1.172822 | -0.857705 | -2.123825 | | H | 1.256786 | -1.634737 | -0.037477 | | H | -0.843801 | -2.379492 | 0.074897 | | H | -3.436281 | 0.33925 | 1.229193 | | H | -3.333587 | -1.42433 | 1.244112 | | H | -3.355263 | -1.493033 | -1.101054 | | H | -3.459089 | 0.268454 | -1.187277 | | H | 1.115938 | 0.348997 | 1.354467 | | H | 0.637563 | 1.880118 | 2.070486 | | H | 0.596381 | 1.756955 | -2.193232 | | H | 1.087736 | 0.268545 | -1.399336 | | H | 0.832793 | 3.026549 | -0.098272 | | H | 2.261023 | 1.977146 | -0.079142 | | O | 2.169193 | -1.963546 | -0.115308 | | B | 3.131357 | -1.061962 | 0.022654 | | O | 4.051199 | -0.264618 | 0.141092 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | 0.497429 | 0.364124 | 0.675806 | | C | 0.463726 | 0.276913 | -0.853881 | | C | 0.963232 | -0.977249 | 1.179198 | | C | 1.006145 | -1.147444 | -1.091224 | | C | 2.001088 | -1.311445 | 0.073897 | | C | -0.121955 | -2.036009 | 0.875596 | | C | -0.105877 | -2.1356 | -0.680839 | | C | 1.076568 | 1.691355 | 1.104385 | | C | 1.324443 | 1.478538 | -1.28872 | | C | 1.065846 | 2.522353 | -0.191369 | | H | -1.384343 | 0.638854 | 1.160588 | | H | -0.542131 | 0.381243 | -1.287327 | | H | 1.330383 | -0.981686 | 2.209871 | | H | 1.404814 | -1.311955 | -2.097553 | | H | 2.842538 | -0.612269 | 0.044206 | | H | 2.392969 | -2.331209 | 0.164186 | | H | -1.098758 | -1.75822 | 1.279716 | | H | 0.156261 | -2.990406 | 1.334099 | | H | 0.143871 | -3.15125 | -1.003456 | | H | -1.068208 | -1.875865 | -1.132033 | | H | 2.108165 | 1.536443 | 1.458533 | | H | 0.533385 | 2.1632 | 1.932326 | | H | 1.067155 | 1.831576 | -2.291924 | | H | 2.384993 | 1.199269 | -1.29467 | | H | 0.075246 | 2.968844 | -0.334616 | | H | 1.798527 | 3.33469 | -0.184171 | | O | -2.359706 | 0.754129 | 1.168158 | | B | -2.923656 | 0.396657 | 0.022903 | | O | -3.459101 | 0.073651 | -1.029332 | | | | |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **vdW2 BO2/R5** | | | | **vdW2 BO2/R6** | | | |
| |  |  |  |  | | --- | --- | --- | --- | | C | 0.232005 | 0.155898 | 0.78197 | | C | 0.202568 | -0.254542 | -0.733478 | | C | 1.750149 | 0.322439 | 1.073321 | | C | 1.698054 | -0.303682 | -1.096 | | C | 2.274444 | 0.857216 | -0.268737 | | C | 2.369102 | -1.08688 | 1.104465 | | C | 2.324952 | -1.521811 | -0.391131 | | C | -0.538874 | 1.436646 | 0.859617 | | C | -0.604844 | 0.837576 | -1.477996 | | C | -0.839172 | 2.006011 | -0.493418 | | H | -0.181415 | -0.615794 | 1.447974 | | H | -0.265108 | -1.23365 | -0.883806 | | H | 1.960842 | 0.928707 | 1.960608 | | H | 1.883768 | -0.271486 | -2.174903 | | H | 1.876965 | 1.839051 | -0.541918 | | H | 3.368972 | 0.901391 | -0.303676 | | H | 1.815275 | -1.764008 | 1.762361 | | H | 3.39912 | -1.042386 | 1.473128 | | H | 3.332333 | -1.712353 | -0.77507 | | H | 1.735612 | -2.429816 | -0.551926 | | H | -0.545075 | 2.046932 | 1.762337 | | H | -2.30947 | 0.510945 | 1.238023 | | H | -1.558864 | 0.420108 | -1.811805 | | H | -0.075149 | 1.170319 | -2.37664 | | H | -1.855205 | 2.415788 | -0.563377 | | H | -0.168247 | 2.85227 | -0.705922 | | O | -3.086456 | -0.080058 | 1.231324 | | B | -3.115787 | -0.911733 | 0.199414 | | O | -3.16926 | -1.688765 | -0.744341 | | | | | |  |  |  |  | | --- | --- | --- | --- | | C | -0.720762 | 0.305292 | 1.143938 | | C | -1.463548 | 1.138442 | 0.036263 | | C | -0.573614 | -1.086552 | 0.4893 | | C | -1.77114 | 0.077428 | -1.03408 | | C | -0.480936 | -0.756511 | -1.011676 | | C | -1.954413 | -1.76346 | 0.544475 | | C | -2.797547 | -0.917374 | -0.456967 | | C | 0.601998 | 1.039164 | 1.436649 | | C | -0.469398 | 2.225049 | -0.440966 | | C | 0.822746 | 1.959497 | 0.273584 | | H | -1.316676 | 0.223728 | 2.06019 | | H | -2.384805 | 1.59775 | 0.413078 | | H | 0.241552 | -1.689119 | 0.902631 | | H | -2.058876 | 0.504165 | -2.001374 | | H | 0.407959 | -0.188832 | -1.295989 | | H | -0.533609 | -1.6511 | -1.642239 | | H | -2.371867 | -1.769434 | 1.556298 | | H | -1.881144 | -2.804645 | 0.213929 | | H | -3.216973 | -1.543895 | -1.250482 | | H | -3.633053 | -0.39904 | 0.025061 | | H | 1.429366 | 0.343775 | 1.628503 | | H | 0.504391 | 1.640313 | 2.355908 | | H | -0.838547 | 3.230815 | -0.188167 | | H | -0.35494 | 2.217422 | -1.533775 | | H | 1.630908 | 2.691556 | 0.269907 | | H | 2.313547 | 0.880688 | -0.790405 | | O | 3.028747 | 0.270043 | -1.041284 | | B | 3.083416 | -0.820381 | -0.286511 | | O | 3.156925 | -1.833555 | 0.394579 | | | | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R1** | | **R2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 150.80 | | ν2 | 178.27 | | ν3 | 276.22 | | ν4 | 305.30 | | ν5 | 329.67 | | ν6 | 385.28 | | ν7 | 468.04 | | ν8 | 496.17 | | ν9 | 550.62 | | ν10 | 575.95 | | ν11 | 668.40 | | ν12 | 758.68 | | ν13 | 780.21 | | ν14 | 814.91 | | ν15 | 880.23 | | ν16 | 884.44 | | ν17 | 914.54 | | ν18 | 924.55 | | ν19 | 930.29 | | ν20 | 941.29 | | ν21 | 956.05 | | ν22 | 960.59 | | ν23 | 984.53 | | ν24 | 1007.97 | | ν25 | 1022.76 | | ν26 | 1037.13 | | ν27 | 1057.54 | | ν28 | 1064.38 | | ν29 | 1075.16 | | ν30 | 1095.46 | | ν31 | 1141.55 | | ν32 | 1163.39 | | ν33 | 1170.34 | | ν34 | 1202.49 | | ν35 | 1215.52 | | ν36 | 1230.44 | | ν37 | 1255.23 | | ν38 | 1271.95 | | ν39 | 1286.16 | | ν40 | 1292.83 | | ν41 | 1306.80 | | ν42 | 1318.04 | | ν43 | 1331.49 | | ν44 | 1341.74 | | ν45 | 1353.46 | | ν46 | 1357.65 | | ν47 | 1362.39 | | ν48 | 1376.53 | | ν49 | 1385.20 | | ν50 | 1511.62 | | ν51 | 1525.26 | | ν52 | 1527.82 | | ν53 | 1537.29 | | ν54 | 1553.92 | | ν55 | 3034.07 | | ν56 | 3074.04 | | ν57 | 3075.12 | | ν58 | 3075.90 | | ν59 | 3076.77 | | ν60 | 3089.05 | | ν61 | 3094.07 | | ν62 | 3096.64 | | ν63 | 3118.32 | | ν64 | 3125.42 | | ν65 | 3130.04 | | ν66 | 3135.61 | | ν67 | 3144.49 | | ν68 | 3159.25 | | ν69 | 3230.98 | | | |  | | --- | | 0.0565 | | 0.1355 | | 3.2021 | | 3.5611 | | 0.0812 | | 3.6049 | | 17.5334 | | 2.2611 | | 0.174 | | 5.5816 | | 0.8415 | | 0.6212 | | 0.5466 | | 1.5443 | | 0.2929 | | 1.6787 | | 0.1984 | | 0.6254 | | 1.8682 | | 1.2883 | | 0.3219 | | 0.1298 | | 2.9519 | | 0.7206 | | 1.445 | | 3.1683 | | 0.121 | | 0.1548 | | 0.1396 | | 0.7303 | | 0.592 | | 0.3808 | | 0.6483 | | 1.5431 | | 0.2356 | | 0.3789 | | 1.6136 | | 1.1613 | | 1.7483 | | 1.9139 | | 0.6116 | | 0.5003 | | 1.3477 | | 1.6207 | | 2.4893 | | 1.1672 | | 0.7739 | | 1.8215 | | 0.4517 | | 4.9085 | | 3.0828 | | 3.857 | | 7.5991 | | 13.0791 | | 39.922 | | 23.7347 | | 34.0002 | | 21.3529 | | 1.0908 | | 11.0864 | | 52.4341 | | 17.4993 | | 52.9796 | | 17.7962 | | 31.4355 | | 29.4332 | | 58.0494 | | 27.6229 | | 22.287 | | |  | | --- | | 135.47 | | 178.27 | | 263.61 | | 316.98 | | 330.64 | | 402.51 | | 494.82 | | 522.67 | | 554.93 | | 662.09 | | 732.11 | | 763.99 | | 802.62 | | 838.60 | | 855.72 | | 878.64 | | 899.11 | | 913.86 | | 934.44 | | 939.16 | | 956.91 | | 976.43 | | 995.74 | | 1022.11 | | 1026.22 | | 1063.26 | | 1071.96 | | 1079.74 | | 1107.09 | | 1127.42 | | 1158.68 | | 1181.18 | | 1212.36 | | 1214.67 | | 1225.81 | | 1236.31 | | 1251.59 | | 1275.49 | | 1282.90 | | 1302.39 | | 1317.08 | | 1321.47 | | 1327.16 | | 1333.56 | | 1348.27 | | 1362.89 | | 1376.43 | | 1390.23 | | 1521.19 | | 1523.26 | | 1528.21 | | 1532.92 | | 1545.21 | | 1556.85 | | 3075.11 | | 3075.39 | | 3078.72 | | 3082.96 | | 3085.10 | | 3094.57 | | 3097.32 | | 3101.15 | | 3111.94 | | 3131.21 | | 3137.53 | | 3138.78 | | 3148.65 | | 3158.39 | | 3170.19 | | |  | | --- | | 0.0973 | | 0.0472 | | 0.2159 | | 0.4626 | | 0.0729 | | 0.0998 | | 0.6943 | | 0.6841 | | 0.553 | | 1.3754 | | 0.1221 | | 0.3684 | | 0.6862 | | 0.6325 | | 5.2264 | | 0.491 | | 0.0932 | | 0.3485 | | 0.0652 | | 2.055 | | 1.9992 | | 1.666 | | 0.7941 | | 0.8302 | | 2.4999 | | 0.2115 | | 0.0572 | | 0.2131 | | 0.2356 | | 0.2747 | | 1.0416 | | 0.396 | | 0.2153 | | 0.5124 | | 4.9354 | | 1.7613 | | 3.2631 | | 0.718 | | 1.1925 | | 2.6855 | | 1.2727 | | 2.0023 | | 1.8236 | | 2.3021 | | 1.207 | | 0.3059 | | 0.5065 | | 0.9305 | | 2.1516 | | 0.3473 | | 3.9478 | | 11.1111 | | 13.0778 | | 8.698 | | 21.2737 | | 33.6201 | | 4.8542 | | 28.5711 | | 17.5351 | | 31.8993 | | 52.7881 | | 24.5497 | | 35.3399 | | 27.5236 | | 4.3181 | | 29.9643 | | 44.6576 | | 49.6916 | | 26.1427 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R3** | | **R4** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 104.16 | | ν2 | 185.23 | | ν3 | 242.11 | | ν4 | 316.87 | | ν5 | 318.54 | | ν6 | 357.53 | | ν7 | 448.13 | | ν8 | 531.13 | | ν9 | 545.67 | | ν10 | 667.53 | | ν11 | 721.19 | | ν12 | 748.05 | | ν13 | 784.07 | | ν14 | 809.50 | | ν15 | 847.58 | | ν16 | 876.58 | | ν17 | 887.72 | | ν18 | 906.08 | | ν19 | 932.43 | | ν20 | 944.46 | | ν21 | 946.02 | | ν22 | 975.61 | | ν23 | 976.18 | | ν24 | 1018.18 | | ν25 | 1023.41 | | ν26 | 1038.80 | | ν27 | 1064.70 | | ν28 | 1071.56 | | ν29 | 1074.56 | | ν30 | 1096.18 | | ν31 | 1172.68 | | ν32 | 1182.00 | | ν33 | 1208.44 | | ν34 | 1214.91 | | ν35 | 1223.76 | | ν36 | 1225.05 | | ν37 | 1249.99 | | ν38 | 1263.31 | | ν39 | 1284.20 | | ν40 | 1285.33 | | ν41 | 1309.40 | | ν42 | 1319.45 | | ν43 | 1323.88 | | ν44 | 1344.33 | | ν45 | 1346.61 | | ν46 | 1362.80 | | ν47 | 1363.35 | | ν48 | 1380.09 | | ν49 | 1381.68 | | ν50 | 1519.61 | | ν51 | 1522.90 | | ν52 | 1525.93 | | ν53 | 1541.13 | | ν54 | 1544.65 | | ν55 | 3071.89 | | ν56 | 3073.20 | | ν57 | 3073.57 | | ν58 | 3073.72 | | ν59 | 3078.72 | | ν60 | 3086.95 | | ν61 | 3089.82 | | ν62 | 3128.11 | | ν63 | 3130.08 | | ν64 | 3132.46 | | ν65 | 3132.82 | | ν66 | 3134.74 | | ν67 | 3144.21 | | ν68 | 3149.73 | | ν69 | 3214.44 | | | |  | | --- | | 0.0054 | | 0.1348 | | 0.0313 | | 0.078 | | 0.7193 | | 5.1519 | | 5.6907 | | 0.7104 | | 1.1932 | | 0.3373 | | 17.1714 | | 1.2071 | | 1.1605 | | 0.9972 | | 1.9684 | | 0.9678 | | 1.0122 | | 0.7601 | | 0.0221 | | 2.5387 | | 0.2079 | | 0.6065 | | 1.8518 | | 2.246 | | 1.485 | | 0.0837 | | 0.0626 | | 0.0748 | | 0.4156 | | 1.2723 | | 0.5595 | | 1.5394 | | 1.5999 | | 0.4279 | | 0.5893 | | 1.104 | | 0.9515 | | 0.7418 | | 2.4545 | | 0.0332 | | 0.0009 | | 0.0107 | | 0.2876 | | 2.2807 | | 0.1505 | | 0.8032 | | 0.4823 | | 3.6908 | | 0.5039 | | 4.8805 | | 1.0547 | | 8.2565 | | 2.9249 | | 8.6682 | | 33.7046 | | 15.9668 | | 0.2394 | | 29.398 | | 32.361 | | 13.7399 | | 76.3336 | | 25.7678 | | 27.7661 | | 0.7636 | | 38.8501 | | 27.0655 | | 44.897 | | 57.6503 | | 21.4684 | | |  | | --- | | 116.76 | | 163.75 | | 236.22 | | 298.48 | | 315.66 | | 389.96 | | 485.76 | | 540.63 | | 557.48 | | 627.20 | | 730.84 | | 752.93 | | 812.34 | | 838.90 | | 865.35 | | 895.37 | | 902.41 | | 915.23 | | 919.73 | | 934.21 | | 946.63 | | 981.35 | | 982.70 | | 1020.37 | | 1034.85 | | 1059.75 | | 1068.51 | | 1077.45 | | 1114.04 | | 1141.99 | | 1147.14 | | 1169.76 | | 1176.75 | | 1208.19 | | 1230.04 | | 1243.23 | | 1250.17 | | 1267.13 | | 1276.32 | | 1289.14 | | 1321.32 | | 1323.00 | | 1330.06 | | 1333.94 | | 1355.97 | | 1357.53 | | 1368.98 | | 1385.34 | | 1508.81 | | 1521.84 | | 1524.58 | | 1531.77 | | 1541.39 | | 1554.17 | | 3022.95 | | 3040.00 | | 3074.05 | | 3080.31 | | 3081.79 | | 3081.97 | | 3092.26 | | 3100.07 | | 3118.08 | | 3130.69 | | 3134.21 | | 3135.49 | | 3144.10 | | 3148.39 | | 3156.58 | | |  | | --- | | 0.118 | | 0.1894 | | 0.2715 | | 0.4033 | | 0.1367 | | 0.0329 | | 0.6848 | | 0.2203 | | 0.8622 | | 3.2183 | | 0.1909 | | 0.3897 | | 1.5299 | | 1.329 | | 0.4765 | | 1.9823 | | 0.509 | | 0.764 | | 0.5235 | | 0.3669 | | 1.4536 | | 0.232 | | 4.5103 | | 1.6645 | | 1.3566 | | 0.2177 | | 0.1557 | | 0.054 | | 2.0984 | | 0.6795 | | 0.077 | | 0.1267 | | 0.628 | | 1.6476 | | 1.535 | | 1.9789 | | 0.797 | | 0.2072 | | 1.1544 | | 1.0156 | | 0.2401 | | 0.2904 | | 1.8542 | | 4.3596 | | 2.0529 | | 0.2455 | | 0.5108 | | 0.7641 | | 4.882 | | 0.8681 | | 1.8937 | | 10.3184 | | 12.7643 | | 3.6726 | | 27.8484 | | 22.3692 | | 12.9793 | | 40.2035 | | 21.9296 | | 21.5085 | | 55.7636 | | 34.0208 | | 50.8464 | | 29.5244 | | 32.1031 | | 8.0411 | | 9.9717 | | 51.6051 | | 42.9328 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R5** | | **R6** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 119.67 | | ν2 | 137.09 | | ν3 | 255.60 | | ν4 | 296.94 | | ν5 | 317.78 | | ν6 | 400.86 | | ν7 | 416.92 | | ν8 | 500.82 | | ν9 | 535.19 | | ν10 | 622.92 | | ν11 | 747.00 | | ν12 | 764.39 | | ν13 | 774.02 | | ν14 | 813.54 | | ν15 | 846.25 | | ν16 | 865.37 | | ν17 | 888.39 | | ν18 | 918.60 | | ν19 | 935.38 | | ν20 | 952.31 | | ν21 | 955.23 | | ν22 | 977.79 | | ν23 | 986.25 | | ν24 | 1006.20 | | ν25 | 1028.10 | | ν26 | 1046.51 | | ν27 | 1064.92 | | ν28 | 1072.04 | | ν29 | 1085.22 | | ν30 | 1097.94 | | ν31 | 1139.79 | | ν32 | 1154.09 | | ν33 | 1177.00 | | ν34 | 1205.45 | | ν35 | 1226.58 | | ν36 | 1235.12 | | ν37 | 1251.63 | | ν38 | 1263.89 | | ν39 | 1291.28 | | ν40 | 1297.64 | | ν41 | 1308.16 | | ν42 | 1316.66 | | ν43 | 1331.37 | | ν44 | 1332.77 | | ν45 | 1337.56 | | ν46 | 1346.72 | | ν47 | 1364.62 | | ν48 | 1377.67 | | ν49 | 1387.79 | | ν50 | 1511.01 | | ν51 | 1525.03 | | ν52 | 1526.88 | | ν53 | 1542.70 | | ν54 | 1554.72 | | ν55 | 3004.31 | | ν56 | 3014.09 | | ν57 | 3079.07 | | ν58 | 3083.14 | | ν59 | 3086.14 | | ν60 | 3088.00 | | ν61 | 3088.98 | | ν62 | 3108.42 | | ν63 | 3113.96 | | ν64 | 3123.04 | | ν65 | 3128.97 | | ν66 | 3141.40 | | ν67 | 3148.40 | | ν68 | 3152.21 | | ν69 | 3222.35 | | | |  | | --- | | 0.0683 | | 0.2673 | | 0.3586 | | 0.6589 | | 0.4154 | | 0.4797 | | 22.4569 | | 0.597 | | 0.2082 | | 0.7574 | | 0.2122 | | 1.9491 | | 1.0861 | | 0.674 | | 0.5372 | | 0.5833 | | 1.7869 | | 0.6405 | | 0.2748 | | 0.1458 | | 1.5834 | | 2.7445 | | 0.4756 | | 1.9206 | | 1.5785 | | 0.1983 | | 0.1531 | | 0.0441 | | 0.3259 | | 1.0807 | | 0.0094 | | 0.3539 | | 1.0117 | | 0.4123 | | 3.9673 | | 0.5261 | | 0.6497 | | 0.1499 | | 1.5752 | | 0.3781 | | 0.4089 | | 0.5451 | | 0.0591 | | 1.933 | | 1.7659 | | 5.3194 | | 0.9899 | | 1.9113 | | 0.7712 | | 2.9537 | | 2.4332 | | 5.0538 | | 14.9919 | | 4.037 | | 39.6552 | | 29.3286 | | 21.9037 | | 13.082 | | 37.6354 | | 14.8897 | | 58.1459 | | 29.3292 | | 65.594 | | 17.8516 | | 1.0162 | | 30.185 | | 58.2285 | | 26.7011 | | 22.3624 | | |  | | --- | | 96.11 | | 116.86 | | 252.25 | | 278.61 | | 325.99 | | 394.14 | | 402.77 | | 499.95 | | 531.09 | | 690.87 | | 703.96 | | 746.09 | | 785.70 | | 810.63 | | 841.15 | | 861.12 | | 914.88 | | 920.74 | | 933.15 | | 952.28 | | 953.68 | | 973.02 | | 987.74 | | 990.58 | | 1040.77 | | 1052.08 | | 1067.31 | | 1074.32 | | 1086.33 | | 1098.08 | | 1150.21 | | 1163.97 | | 1164.17 | | 1203.35 | | 1220.26 | | 1231.93 | | 1255.07 | | 1267.83 | | 1288.24 | | 1297.61 | | 1311.85 | | 1322.68 | | 1326.88 | | 1334.64 | | 1335.25 | | 1365.77 | | 1368.84 | | 1378.67 | | 1391.91 | | 1510.27 | | 1512.70 | | 1525.31 | | 1535.43 | | 1555.06 | | 3000.43 | | 3001.66 | | 3078.22 | | 3079.60 | | 3082.85 | | 3084.31 | | 3088.78 | | 3095.19 | | 3105.14 | | 3112.49 | | 3118.55 | | 3129.12 | | 3144.45 | | 3148.97 | | 3228.34 | | |  | | --- | | 0.6883 | | 0.0028 | | 0.0102 | | 0.9791 | | 0.0043 | | 25.9986 | | 2.3727 | | 0.238 | | 0.0243 | | 1.0594 | | 0.5126 | | 0.3311 | | 0.0258 | | 0.8901 | | 1.0587 | | 0.9222 | | 1.7527 | | 0.3797 | | 1.2003 | | 1.303 | | 0.138 | | 1.4825 | | 0.4554 | | 2.1979 | | 2.2594 | | 0.0364 | | 0.6004 | | 0.2662 | | 0.0803 | | 0.0279 | | 0.7594 | | 0 | | 1.2014 | | 0.7623 | | 0.0001 | | 2.394 | | 2.0392 | | 0.0303 | | 0.8217 | | 0.3828 | | 0.1835 | | 0.0186 | | 0.2238 | | 0.2796 | | 5.7763 | | 0.3518 | | 4.6962 | | 0.4934 | | 0.6535 | | 6.8327 | | 1.9299 | | 1.5708 | | 16.2584 | | 4.6516 | | 30.893 | | 22.8575 | | 12.7894 | | 7.5315 | | 19.3657 | | 18.1288 | | 53.0711 | | 33.6013 | | 61.5819 | | 77.948 | | 2.9792 | | 0.0418 | | 23.2414 | | 61.8299 | | 30.3967 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **JP-10 B3LYP/def2-TZVP** | |  | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 144.86 | | ν2 | 183.19 | | ν3 | 278.68 | | ν4 | 323.98 | | ν5 | 331.23 | | ν6 | 406.96 | | ν7 | 505.76 | | ν8 | 538.22 | | ν9 | 562.37 | | ν10 | 677.86 | | ν11 | 742.45 | | ν12 | 759.89 | | ν13 | 794.65 | | ν14 | 835.78 | | ν15 | 869.43 | | ν16 | 870.56 | | ν17 | 891.40 | | ν18 | 899.24 | | ν19 | 916.88 | | ν20 | 924.82 | | ν21 | 927.57 | | ν22 | 961.72 | | ν23 | 965.13 | | ν24 | 994.87 | | ν25 | 1004.67 | | ν26 | 1047.38 | | ν27 | 1055.60 | | ν28 | 1057.47 | | ν29 | 1058.01 | | ν30 | 1080.23 | | ν31 | 1140.77 | | ν32 | 1157.37 | | ν33 | 1173.26 | | ν34 | 1193.87 | | ν35 | 1207.72 | | ν36 | 1214.09 | | ν37 | 1232.45 | | ν38 | 1254.23 | | ν39 | 1264.61 | | ν40 | 1293.87 | | ν41 | 1303.64 | | ν42 | 1309.67 | | ν43 | 1316.68 | | ν44 | 1321.65 | | ν45 | 1331.83 | | ν46 | 1334.48 | | ν47 | 1348.14 | | ν48 | 1353.50 | | ν49 | 1373.56 | | ν50 | 1377.82 | | ν51 | 1494.18 | | ν52 | 1497.05 | | ν53 | 1499.72 | | ν54 | 1505.95 | | ν55 | 1516.87 | | ν56 | 1531.63 | | ν57 | 3018.20 | | ν58 | 3024.48 | | ν59 | 3027.22 | | ν60 | 3033.56 | | ν61 | 3038.18 | | ν62 | 3046.39 | | ν63 | 3047.55 | | ν64 | 3049.67 | | ν65 | 3067.56 | | ν66 | 3070.81 | | ν67 | 3074.56 | | ν68 | 3077.32 | | ν69 | 3080.47 | | ν70 | 3083.92 | | ν71 | 3091.25 | | ν72 | 3092.16 | | | |  | | --- | | 0.009 | | 0.0031 | | 0.0817 | | 0.0513 | | 0.0421 | | 0.0462 | | 0.2251 | | 0.1734 | | 0.5638 | | 0.524 | | 0.3066 | | 0.3185 | | 1.3279 | | 0.5303 | | 1.0147 | | 0.0155 | | 0.6079 | | 0.0652 | | 0.9298 | | 0.077 | | 1.1053 | | 1.7838 | | 0.0305 | | 1.6714 | | 0.489 | | 0.2149 | | 0.6282 | | 0.0282 | | 0.0489 | | 0.5847 | | 0.1199 | | 0.0264 | | 1.0062 | | 0.2069 | | 0.0662 | | 1.3373 | | 1.2409 | | 0.0055 | | 0.7579 | | 1.2094 | | 0.0343 | | 0.2175 | | 0.412 | | 0.0001 | | 0.0798 | | 1.6902 | | 0.5566 | | 0.9748 | | 0.7613 | | 0.4264 | | 1.123 | | 1.8945 | | 1.9952 | | 4.2672 | | 10.7064 | | 4.8919 | | 20.496 | | 29.4339 | | 19.6381 | | 1.1218 | | 24.6142 | | 55.0985 | | 8.1301 | | 72.3811 | | 6.2772 | | 44.6458 | | 41.3424 | | 97.7589 | | 45.9135 | | 10.4729 | | 82.9497 | | 50.3735 | |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R1 B3LYP/def2-TZVP** | | **R2 B3LYP/def2-TZVP** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 154.52 | | ν2 | 179.74 | | ν3 | 269.30 | | ν4 | 304.29 | | ν5 | 328.29 | | ν6 | 377.36 | | ν7 | 444.94 | | ν8 | 506.69 | | ν9 | 553.10 | | ν10 | 573.17 | | ν11 | 677.19 | | ν12 | 747.23 | | ν13 | 768.85 | | ν14 | 795.54 | | ν15 | 866.58 | | ν16 | 869.54 | | ν17 | 891.38 | | ν18 | 904.31 | | ν19 | 913.76 | | ν20 | 916.62 | | ν21 | 934.59 | | ν22 | 936.76 | | ν23 | 960.23 | | ν24 | 981.98 | | ν25 | 998.40 | | ν26 | 1011.99 | | ν27 | 1035.93 | | ν28 | 1045.81 | | ν29 | 1053.22 | | ν30 | 1074.12 | | ν31 | 1122.61 | | ν32 | 1145.38 | | ν33 | 1159.77 | | ν34 | 1188.11 | | ν35 | 1193.46 | | ν36 | 1212.58 | | ν37 | 1234.56 | | ν38 | 1252.49 | | ν39 | 1272.05 | | ν40 | 1283.11 | | ν41 | 1300.32 | | ν42 | 1307.81 | | ν43 | 1319.44 | | ν44 | 1327.68 | | ν45 | 1337.67 | | ν46 | 1346.14 | | ν47 | 1347.44 | | ν48 | 1361.57 | | ν49 | 1372.57 | | ν50 | 1473.41 | | ν51 | 1494.66 | | ν52 | 1499.43 | | ν53 | 1508.59 | | ν54 | 1525.09 | | ν55 | 2967.58 | | ν56 | 3010.11 | | ν57 | 3019.34 | | ν58 | 3026.04 | | ν59 | 3029.27 | | ν60 | 3039.33 | | ν61 | 3054.03 | | ν62 | 3055.90 | | ν63 | 3071.17 | | ν64 | 3076.30 | | ν65 | 3083.17 | | ν66 | 3084.22 | | ν67 | 3087.96 | | ν68 | 3097.24 | | ν69 | 3196.12 | | | |  | | --- | | 0.0815 | | 0.1742 | | 7.1892 | | 2.3774 | | 0.0587 | | 5.8178 | | 14.5213 | | 0.503 | | 0.0862 | | 3.5614 | | 0.4164 | | 0.6745 | | 0.2578 | | 1.5931 | | 0.5031 | | 0.2943 | | 0.5595 | | 1.3591 | | 0.6825 | | 0.5315 | | 0.1724 | | 0.2314 | | 2.2927 | | 0.7657 | | 1.0491 | | 1.1601 | | 0.0162 | | 0.87 | | 0.014 | | 0.716 | | 0.4333 | | 0.2268 | | 0.6362 | | 0.597 | | 0.3524 | | 0.1555 | | 1.1736 | | 0.8133 | | 0.4255 | | 1.9975 | | 0.1951 | | 0.1164 | | 0.5644 | | 0.4021 | | 1.5205 | | 0.5283 | | 0.6114 | | 1.1002 | | 0.3848 | | 4.1523 | | 2.2168 | | 2.8636 | | 4.6117 | | 8.8149 | | 46.9071 | | 25.6347 | | 21.4738 | | 29.8635 | | 22.6579 | | 7.4462 | | 42.901 | | 18.2456 | | 38.4271 | | 43.1507 | | 77.8015 | | 93.2132 | | 4.722 | | 32.9053 | | 21.3324 | | |  | | --- | | 144.65 | | 181.25 | | 277.96 | | 321.93 | | 329.63 | | 404.89 | | 502.13 | | 526.28 | | 559.77 | | 668.25 | | 716.25 | | 755.95 | | 773.22 | | 830.80 | | 837.16 | | 858.47 | | 875.94 | | 886.36 | | 913.01 | | 921.73 | | 931.59 | | 950.69 | | 971.47 | | 995.61 | | 1007.00 | | 1042.38 | | 1052.47 | | 1065.04 | | 1087.08 | | 1100.16 | | 1143.07 | | 1166.20 | | 1190.35 | | 1199.66 | | 1212.04 | | 1219.35 | | 1236.52 | | 1255.45 | | 1264.39 | | 1290.15 | | 1303.74 | | 1311.10 | | 1315.93 | | 1322.15 | | 1336.45 | | 1347.68 | | 1364.89 | | 1375.72 | | 1492.06 | | 1493.09 | | 1497.95 | | 1502.77 | | 1514.00 | | 1526.60 | | 3019.50 | | 3028.39 | | 3036.56 | | 3040.21 | | 3042.05 | | 3050.66 | | 3055.79 | | 3058.66 | | 3071.46 | | 3074.56 | | 3077.44 | | 3078.55 | | 3087.58 | | 3098.93 | | 3109.20 | | |  | | --- | | 0.0886 | | 0.0512 | | 0.3358 | | 0.3858 | | 0.0731 | | 0.0916 | | 0.6129 | | 0.7013 | | 0.5547 | | 1.0893 | | 0.1597 | | 0.2605 | | 0.646 | | 0.453 | | 3.4844 | | 0.4177 | | 0.2142 | | 0.3154 | | 1.7382 | | 0.254 | | 1.1531 | | 1.4763 | | 0.5595 | | 0.8167 | | 1.632 | | 0.5466 | | 0.1851 | | 0.1349 | | 0.1698 | | 0.1386 | | 1.0528 | | 0.149 | | 0.1553 | | 0.5433 | | 4.2047 | | 1.5739 | | 1.5887 | | 0.9149 | | 0.6344 | | 1.6759 | | 0.7396 | | 0.3102 | | 0.8326 | | 1.2636 | | 0.4335 | | 0.2288 | | 0.4053 | | 0.6912 | | 1.5808 | | 0.3995 | | 2.5398 | | 6.6318 | | 8.3847 | | 5.8937 | | 25.6647 | | 25.7544 | | 16.9318 | | 14.0374 | | 14.3771 | | 47.6343 | | 51.4164 | | 24.7223 | | 44.1276 | | 32.5003 | | 56.9166 | | 9.3664 | | 51.0083 | | 72.6197 | | 32.3534 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R3 B3LYP/def2-TZVP** | | **R4 B3LYP/def2-TZVP** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 111.86 | | ν2 | 187.42 | | ν3 | 261.45 | | ν4 | 308.49 | | ν5 | 321.25 | | ν6 | 337.24 | | ν7 | 429.89 | | ν8 | 535.22 | | ν9 | 548.59 | | ν10 | 674.72 | | ν11 | 675.02 | | ν12 | 739.90 | | ν13 | 768.83 | | ν14 | 794.66 | | ν15 | 836.73 | | ν16 | 855.58 | | ν17 | 872.73 | | ν18 | 878.33 | | ν19 | 914.40 | | ν20 | 919.24 | | ν21 | 928.82 | | ν22 | 948.99 | | ν23 | 950.47 | | ν24 | 991.11 | | ν25 | 994.38 | | ν26 | 998.52 | | ν27 | 1041.85 | | ν28 | 1052.21 | | ν29 | 1058.98 | | ν30 | 1078.17 | | ν31 | 1156.48 | | ν32 | 1167.36 | | ν33 | 1191.32 | | ν34 | 1192.74 | | ν35 | 1208.06 | | ν36 | 1208.95 | | ν37 | 1239.71 | | ν38 | 1244.86 | | ν39 | 1263.13 | | ν40 | 1277.97 | | ν41 | 1299.40 | | ν42 | 1309.49 | | ν43 | 1316.00 | | ν44 | 1333.44 | | ν45 | 1333.73 | | ν46 | 1348.42 | | ν47 | 1348.92 | | ν48 | 1369.20 | | ν49 | 1372.65 | | ν50 | 1489.88 | | ν51 | 1493.07 | | ν52 | 1493.30 | | ν53 | 1508.94 | | ν54 | 1513.37 | | ν55 | 3015.69 | | ν56 | 3020.86 | | ν57 | 3024.86 | | ν58 | 3033.21 | | ν59 | 3036.58 | | ν60 | 3045.15 | | ν61 | 3050.22 | | ν62 | 3069.62 | | ν63 | 3071.10 | | ν64 | 3074.48 | | ν65 | 3082.09 | | ν66 | 3090.87 | | ν67 | 3094.27 | | ν68 | 3097.54 | | ν69 | 3190.92 | | | |  | | --- | | 0.0013 | | 0.1451 | | 0.0526 | | 2.5297 | | 0.0591 | | 8.1255 | | 4.7033 | | 0.5368 | | 0.9172 | | 13.1661 | | 0.1795 | | 1.2947 | | 0.5191 | | 0.812 | | 1.476 | | 0.3368 | | 0.1344 | | 1.0743 | | 0.0633 | | 1.9664 | | 0.0444 | | 0.1656 | | 1.5318 | | 1.5685 | | 0.151 | | 0.991 | | 0.154 | | 0.1074 | | 0.1418 | | 0.6567 | | 0.407 | | 1.1113 | | 0.2743 | | 0.9488 | | 0.3175 | | 0.2456 | | 1.0744 | | 0.1264 | | 1.5503 | | 0.0017 | | 0.0179 | | 0.2732 | | 0.0038 | | 0.8227 | | 0.0987 | | 0.549 | | 0.3872 | | 1.9851 | | 0.3784 | | 3.4971 | | 0.5015 | | 5.8954 | | 2.6721 | | 5.2584 | | 19.1536 | | 30.4691 | | 25.7237 | | 7.9221 | | 26.3054 | | 22.3585 | | 80.6865 | | 0.05 | | 39.3357 | | 51.8496 | | 58.3304 | | 53.6016 | | 73.0037 | | 20.462 | | 17.6983 | | |  | | --- | | 116.60 | | 161.82 | | 239.56 | | 291.98 | | 316.28 | | 390.16 | | 494.61 | | 542.14 | | 561.15 | | 628.85 | | 723.59 | | 740.35 | | 795.26 | | 831.53 | | 849.30 | | 876.57 | | 882.40 | | 890.91 | | 896.22 | | 907.04 | | 917.41 | | 957.27 | | 964.24 | | 990.06 | | 1019.21 | | 1040.19 | | 1047.23 | | 1062.80 | | 1095.04 | | 1124.00 | | 1133.89 | | 1152.89 | | 1166.31 | | 1190.56 | | 1208.27 | | 1224.14 | | 1234.37 | | 1249.11 | | 1252.67 | | 1285.78 | | 1305.34 | | 1311.16 | | 1315.06 | | 1326.56 | | 1339.45 | | 1342.06 | | 1353.64 | | 1366.69 | | 1470.83 | | 1492.19 | | 1493.11 | | 1502.73 | | 1509.56 | | 1526.23 | | 2953.46 | | 2983.86 | | 3018.23 | | 3025.50 | | 3036.07 | | 3038.69 | | 3038.99 | | 3050.10 | | 3073.37 | | 3074.21 | | 3083.28 | | 3084.07 | | 3088.13 | | 3093.95 | | 3097.42 | | |  | | --- | | 0.1225 | | 0.1459 | | 0.4748 | | 0.3404 | | 0.0869 | | 0.0281 | | 0.5806 | | 0.1624 | | 1.0262 | | 3.203 | | 0.1385 | | 0.2311 | | 2.1631 | | 0.7287 | | 0.1588 | | 0.8024 | | 0.6114 | | 0.2136 | | 0.7737 | | 0.2267 | | 0.915 | | 0.018 | | 2.8843 | | 1.1328 | | 0.2754 | | 0.0326 | | 1.0466 | | 0.2034 | | 1.1335 | | 0.3732 | | 0.2313 | | 0.2065 | | 0.6413 | | 1.7135 | | 1.4261 | | 0.9616 | | 0.3267 | | 0.2375 | | 0.6844 | | 1.0408 | | 0.4388 | | 0.2227 | | 0.4198 | | 1.5901 | | 0.3495 | | 1.0895 | | 0.0348 | | 0.2754 | | 3.8874 | | 1.2989 | | 1.6532 | | 3.198 | | 9.2603 | | 3.2276 | | 34.79 | | 26.3467 | | 19.0731 | | 11.6416 | | 55.6529 | | 26.2375 | | 42.3396 | | 64.2788 | | 2.7039 | | 64.1029 | | 23.1515 | | 70.1505 | | 45.8074 | | 20.2313 | | 60.2549 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R5 B3LYP/def2-TZVP** | | **R6 B3LYP/def2-TZVP** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 120.90 | | ν2 | 133.95 | | ν3 | 267.23 | | ν4 | 290.21 | | ν5 | 319.78 | | ν6 | 401.50 | | ν7 | 418.33 | | ν8 | 507.86 | | ν9 | 538.59 | | ν10 | 629.92 | | ν11 | 740.16 | | ν12 | 755.04 | | ν13 | 767.56 | | ν14 | 799.35 | | ν15 | 836.68 | | ν16 | 850.60 | | ν17 | 873.21 | | ν18 | 889.38 | | ν19 | 909.53 | | ν20 | 925.48 | | ν21 | 927.62 | | ν22 | 951.88 | | ν23 | 963.46 | | ν24 | 980.57 | | ν25 | 1004.68 | | ν26 | 1021.03 | | ν27 | 1051.39 | | ν28 | 1053.92 | | ν29 | 1066.83 | | ν30 | 1077.31 | | ν31 | 1124.62 | | ν32 | 1145.43 | | ν33 | 1163.19 | | ν34 | 1187.08 | | ν35 | 1210.78 | | ν36 | 1220.17 | | ν37 | 1231.70 | | ν38 | 1247.32 | | ν39 | 1281.70 | | ν40 | 1287.27 | | ν41 | 1295.52 | | ν42 | 1301.97 | | ν43 | 1314.32 | | ν44 | 1320.90 | | ν45 | 1324.06 | | ν46 | 1335.12 | | ν47 | 1349.92 | | ν48 | 1364.35 | | ν49 | 1372.84 | | ν50 | 1471.01 | | ν51 | 1496.30 | | ν52 | 1497.93 | | ν53 | 1510.55 | | ν54 | 1524.97 | | ν55 | 2916.75 | | ν56 | 2951.25 | | ν57 | 3027.39 | | ν58 | 3037.95 | | ν59 | 3043.45 | | ν60 | 3046.67 | | ν61 | 3047.88 | | ν62 | 3049.81 | | ν63 | 3067.07 | | ν64 | 3079.13 | | ν65 | 3081.46 | | ν66 | 3087.65 | | ν67 | 3091.66 | | ν68 | 3092.51 | | ν69 | 3180.15 | | | |  | | --- | | 0.1143 | | 0.2081 | | 0.6456 | | 0.6426 | | 0.4363 | | 3.0735 | | 18.4598 | | 0.6899 | | 0.1126 | | 0.6461 | | 0.0986 | | 1.5252 | | 0.7481 | | 0.7287 | | 0.3308 | | 0.4925 | | 0.8881 | | 0.6722 | | 0.3198 | | 0.1109 | | 1.3552 | | 1.373 | | 0.1667 | | 1.6358 | | 0.8729 | | 0.3603 | | 0.3015 | | 0.2798 | | 0.3804 | | 0.9804 | | 0.0424 | | 0.2195 | | 0.7098 | | 0.2985 | | 2.7293 | | 0.3924 | | 0.8385 | | 0.0552 | | 0.4092 | | 1.3514 | | 0.0518 | | 0.4031 | | 0.291 | | 0.5354 | | 1.4645 | | 2.6536 | | 0.6291 | | 0.9604 | | 1.054 | | 2.2939 | | 1.0639 | | 2.9445 | | 11.4606 | | 3.0114 | | 47.5025 | | 36.524 | | 26.0106 | | 26.8405 | | 24.5827 | | 61.0348 | | 31.953 | | 32.8158 | | 4.955 | | 54.3734 | | 63.1313 | | 20.263 | | 65.3797 | | 39.0635 | | 22.9516 | | |  | | --- | | 83.3286 | | 127.021 | | 265.134 | | 278.9338 | | 329.4545 | | 393.905 | | 405.1738 | | 511.1193 | | 536.0017 | | 687.9005 | | 711.3315 | | 733.6506 | | 772.9638 | | 799.0063 | | 833.6046 | | 843.2213 | | 890.3232 | | 895.0157 | | 913.112 | | 926.8657 | | 937.1678 | | 952.9848 | | 965.6014 | | 967.5085 | | 1016.724 | | 1025.347 | | 1048.893 | | 1057.725 | | 1064.171 | | 1080.183 | | 1134.295 | | 1147.262 | | 1151.437 | | 1180.725 | | 1201.713 | | 1217.232 | | 1236.958 | | 1252.339 | | 1269.27 | | 1294.831 | | 1306.422 | | 1308.093 | | 1311.509 | | 1322.565 | | 1329.05 | | 1348.758 | | 1355.671 | | 1366.202 | | 1379.298 | | 1471.471 | | 1473.821 | | 1494.006 | | 1509.049 | | 1529.677 | | 2924.335 | | 2926.529 | | 3003.138 | | 3003.252 | | 3037.463 | | 3045.19 | | 3048.151 | | 3048.603 | | 3064.499 | | 3067.151 | | 3077.834 | | 3084.06 | | 3086.597 | | 3091.189 | | 3183.43 | | |  | | --- | | 0.7531 | | 0.0001 | | 0.0173 | | 0.8025 | | 0.0017 | | 26.4158 | | 0.3165 | | 0.1762 | | 0.0074 | | 0.6149 | | 0.3173 | | 0.269 | | 0.07 | | 0.9518 | | 0.7728 | | 0.3718 | | 0.5409 | | 0.8602 | | 1.087 | | 1.072 | | 0.6358 | | 0.6736 | | 0.0583 | | 1.422 | | 1.7597 | | 0.0102 | | 0.5321 | | 0.6523 | | 0.5682 | | 0.0102 | | 0.48 | | 0.7383 | | 0.1079 | | 0.5952 | | 0.0212 | | 1.1894 | | 1.3549 | | 0.0015 | | 0.0068 | | 0.9459 | | 0.3764 | | 0.1973 | | 0.2552 | | 0.264 | | 2.4189 | | 0.0892 | | 2.4239 | | 0.0777 | | 0.9583 | | 6.1364 | | 2.0765 | | 1.0736 | | 8.826 | | 4.1653 | | 33.6158 | | 30.7142 | | 35.8921 | | 20.2755 | | 19.2909 | | 39.8441 | | 50.7679 | | 20.2586 | | 52.0511 | | 10.2821 | | 83.6528 | | 2.7467 | | 27.5414 | | 86.8256 | | 30.2786 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 1-2 JP-10/AlO** | | **vdW1 Site 3 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 17.00 | | ν2 | 35.15 | | ν3 | 49.13 | | ν4 | 55.59 | | ν5 | 87.80 | | ν6 | 134.82 | | ν7 | 180.82 | | ν8 | 264.48 | | ν9 | 318.16 | | ν10 | 332.61 | | ν11 | 403.97 | | ν12 | 494.40 | | ν13 | 535.14 | | ν14 | 556.78 | | ν15 | 667.99 | | ν16 | 739.50 | | ν17 | 750.36 | | ν18 | 767.11 | | ν19 | 813.37 | | ν20 | 846.27 | | ν21 | 881.30 | | ν22 | 882.73 | | ν23 | 911.22 | | ν24 | 917.71 | | ν25 | 938.81 | | ν26 | 941.44 | | ν27 | 947.30 | | ν28 | 982.98 | | ν29 | 992.96 | | ν30 | 1020.81 | | ν31 | 1029.20 | | ν32 | 1066.78 | | ν33 | 1069.90 | | ν34 | 1076.44 | | ν35 | 1078.65 | | ν36 | 1096.24 | | ν37 | 1157.96 | | ν38 | 1164.44 | | ν39 | 1186.39 | | ν40 | 1216.15 | | ν41 | 1219.50 | | ν42 | 1228.48 | | ν43 | 1243.29 | | ν44 | 1268.65 | | ν45 | 1284.31 | | ν46 | 1288.98 | | ν47 | 1307.00 | | ν48 | 1321.88 | | ν49 | 1327.59 | | ν50 | 1330.50 | | ν51 | 1340.76 | | ν52 | 1344.29 | | ν53 | 1362.50 | | ν54 | 1364.98 | | ν55 | 1381.74 | | ν56 | 1386.63 | | ν57 | 1522.53 | | ν58 | 1525.60 | | ν59 | 1527.57 | | ν60 | 1533.16 | | ν61 | 1547.12 | | ν62 | 1557.41 | | ν63 | 3066.81 | | ν64 | 3070.91 | | ν65 | 3073.99 | | ν66 | 3074.45 | | ν67 | 3076.02 | | ν68 | 3083.44 | | ν69 | 3087.14 | | ν70 | 3089.62 | | ν71 | 3097.27 | | ν72 | 3116.84 | | ν73 | 3130.13 | | ν74 | 3134.06 | | ν75 | 3135.58 | | ν76 | 3138.22 | | ν77 | 3145.96 | | ν78 | 3156.11 | | | |  | | --- | | 0.4753 | | 1.1885 | | 0.0313 | | 8.5907 | | 11.4418 | | 0.1075 | | 0.1409 | | 0.1635 | | 0.1256 | | 0.5765 | | 0.3471 | | 1.2699 | | 0.687 | | 0.1874 | | 1.0001 | | 189.6392 | | 0.4272 | | 1.3633 | | 1.2643 | | 1.0181 | | 1.2427 | | 3.5929 | | 0.3099 | | 0.5921 | | 0.3408 | | 1.8559 | | 3.4493 | | 4.0438 | | 1.1196 | | 2.166 | | 2.1967 | | 0.8177 | | 0.5057 | | 0.2632 | | 0.3722 | | 0.4668 | | 0.4134 | | 1.4713 | | 2.2199 | | 0.281 | | 2.4034 | | 3.9328 | | 1.8996 | | 0.222 | | 1.4462 | | 3.4556 | | 0.066 | | 0.2783 | | 0.5068 | | 2.3581 | | 4.2183 | | 4.6308 | | 0.6689 | | 2.0614 | | 1.4265 | | 0.5141 | | 1.3694 | | 1.285 | | 2.7122 | | 13.3134 | | 16.0041 | | 5.2029 | | 12.7887 | | 20.8058 | | 12.2776 | | 14.9103 | | 36.9065 | | 15.6569 | | 130.3601 | | 32.5941 | | 81.3895 | | 29.8883 | | 43.7406 | | 29.6455 | | 4.2558 | | 12.7946 | | 53.4531 | | 45.7328 | | |  | | --- | | 22.26 | | 23.90 | | 64.50 | | 76.93 | | 89.36 | | 137.31 | | 187.66 | | 261.39 | | 318.91 | | 337.33 | | 407.11 | | 506.61 | | 532.81 | | 556.83 | | 670.24 | | 754.67 | | 767.97 | | 811.64 | | 844.24 | | 885.61 | | 886.59 | | 918.26 | | 922.32 | | 943.71 | | 944.17 | | 951.38 | | 984.48 | | 997.62 | | 1019.01 | | 1031.76 | | 1068.78 | | 1069.18 | | 1074.08 | | 1075.27 | | 1095.05 | | 1163.26 | | 1180.14 | | 1181.75 | | 1210.22 | | 1225.19 | | 1226.55 | | 1245.04 | | 1270.61 | | 1292.52 | | 1297.17 | | 1309.35 | | 1317.40 | | 1325.13 | | 1338.42 | | 1351.03 | | 1360.10 | | 1364.78 | | 1366.21 | | 1390.27 | | 1391.94 | | 1520.36 | | 1523.42 | | 1529.71 | | 1536.86 | | 1547.15 | | 1576.79 | | 3053.91 | | 3056.53 | | 3064.41 | | 3069.02 | | 3069.14 | | 3077.52 | | 3078.68 | | 3079.65 | | 3102.67 | | 3106.70 | | 3117.71 | | 3118.16 | | 3138.34 | | 3148.64 | | 3149.64 | | 3163.34 | | 4661.83 | | |  | | --- | | 40.7366 | | 43.2182 | | 21.057 | | 17.9013 | | 20.229 | | 0.0738 | | 0.5789 | | 0.0542 | | 0.069 | | 0.8012 | | 0.3409 | | 2.5179 | | 0.1998 | | 0.3803 | | 1.8832 | | 0.2978 | | 0.4537 | | 1.9791 | | 1.4032 | | 0.2994 | | 3.4096 | | 1.0571 | | 0.2979 | | 2.2284 | | 0.6643 | | 0.7174 | | 1.0347 | | 5.9699 | | 3.1737 | | 2.1451 | | 1.5294 | | 0.2915 | | 0.3362 | | 0.503 | | 1.8937 | | 0.0997 | | 1.8224 | | 2.1879 | | 0.4979 | | 0.0252 | | 1.7454 | | 3.1783 | | 0.358 | | 3.5423 | | 0.5519 | | 0.2272 | | 0.4321 | | 1.8959 | | 0.147 | | 0.8046 | | 18.9673 | | 1.739 | | 3.0975 | | 15.9302 | | 0.0243 | | 3.1699 | | 1.3134 | | 0.2951 | | 18.1104 | | 0.4491 | | 34.3308 | | 2.336 | | 468.1902 | | 1254.6599 | | 22.5979 | | 143.156 | | 105.2997 | | 1396.5983 | | 85.9813 | | 128.511 | | 741.8283 | | 0.5857 | | 50.9124 | | 82.4097 | | 2513.5143 | | 5.9911 | | 52.8704 | | 2192532.61 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 4 JP-10/AlO** | | **vdW1 Site 5-6 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 11.82 | | ν2 | 20.20 | | ν3 | 32.24 | | ν4 | 52.90 | | ν5 | 73.20 | | ν6 | 130.81 | | ν7 | 182.22 | | ν8 | 261.41 | | ν9 | 319.49 | | ν10 | 331.98 | | ν11 | 403.48 | | ν12 | 491.99 | | ν13 | 534.03 | | ν14 | 549.35 | | ν15 | 555.16 | | ν16 | 664.43 | | ν17 | 750.26 | | ν18 | 767.90 | | ν19 | 812.32 | | ν20 | 846.11 | | ν21 | 880.04 | | ν22 | 881.38 | | ν23 | 913.06 | | ν24 | 923.50 | | ν25 | 939.24 | | ν26 | 941.42 | | ν27 | 953.82 | | ν28 | 980.84 | | ν29 | 983.76 | | ν30 | 1019.63 | | ν31 | 1030.86 | | ν32 | 1066.86 | | ν33 | 1068.73 | | ν34 | 1076.84 | | ν35 | 1086.14 | | ν36 | 1093.51 | | ν37 | 1147.93 | | ν38 | 1165.40 | | ν39 | 1191.20 | | ν40 | 1212.34 | | ν41 | 1218.95 | | ν42 | 1226.42 | | ν43 | 1242.53 | | ν44 | 1270.29 | | ν45 | 1287.03 | | ν46 | 1288.95 | | ν47 | 1300.35 | | ν48 | 1322.94 | | ν49 | 1328.06 | | ν50 | 1330.62 | | ν51 | 1338.17 | | ν52 | 1340.07 | | ν53 | 1359.76 | | ν54 | 1361.92 | | ν55 | 1394.97 | | ν56 | 1397.68 | | ν57 | 1516.74 | | ν58 | 1520.74 | | ν59 | 1525.99 | | ν60 | 1529.52 | | ν61 | 1542.75 | | ν62 | 1553.73 | | ν63 | 3063.31 | | ν64 | 3063.37 | | ν65 | 3067.62 | | ν66 | 3069.95 | | ν67 | 3077.27 | | ν68 | 3079.84 | | ν69 | 3097.51 | | ν70 | 3103.36 | | ν71 | 3111.86 | | ν72 | 3112.71 | | ν73 | 3127.68 | | ν74 | 3129.03 | | ν75 | 3136.03 | | ν76 | 3143.02 | | ν77 | 3153.09 | | ν78 | 3166.08 | | | |  | | --- | | 38.9297 | | 27.8923 | | 0.041 | | 10.2654 | | 33.5366 | | 0.0085 | | 3.0835 | | 0.0428 | | 0.0316 | | 33.427 | | 110.8308 | | 46.0165 | | 0.2413 | | 9303.529 | | 526.3659 | | 0.6812 | | 0.2219 | | 5.8968 | | 0.0653 | | 6.2705 | | 2.9536 | | 0.6856 | | 0.0055 | | 0.5528 | | 0.1871 | | 1.1771 | | 1.9217 | | 4.138 | | 0.4794 | | 2.2591 | | 2.0966 | | 0.2361 | | 2.2548 | | 0.0542 | | 0.1006 | | 0.6018 | | 0.1518 | | 0.0213 | | 27.0206 | | 0.0018 | | 0.2744 | | 11.4189 | | 8.0718 | | 0.0004 | | 0.4431 | | 0.7887 | | 0.479 | | 0.0307 | | 3.0928 | | 0.8392 | | 2.6104 | | 41.0957 | | 0.3751 | | 15.6515 | | 3.2885 | | 2.4414 | | 0.0155 | | 8.33 | | 2.7749 | | 10.3174 | | 19.3734 | | 45.4829 | | 36.366 | | 30.0372 | | 20.0712 | | 48.7322 | | 49.742 | | 69.4691 | | 103.6163 | | 149.4729 | | 1.4538 | | 74.9856 | | 6.0018 | | 73.3502 | | 121.7255 | | 104.1185 | | 18.1559 | | 104.5249 | | |  | | --- | | 13.05 | | 16.49 | | 32.34 | | 46.63 | | 68.05 | | 128.95 | | 187.74 | | 260.68 | | 318.52 | | 331.21 | | 402.78 | | 491.51 | | 532.43 | | 550.50 | | 638.60 | | 667.04 | | 750.11 | | 767.86 | | 812.23 | | 844.69 | | 881.33 | | 886.07 | | 915.13 | | 918.12 | | 940.29 | | 941.84 | | 952.73 | | 980.72 | | 984.10 | | 1018.45 | | 1033.29 | | 1063.61 | | 1073.19 | | 1074.11 | | 1079.26 | | 1094.83 | | 1149.57 | | 1166.92 | | 1183.86 | | 1213.92 | | 1220.64 | | 1222.99 | | 1244.95 | | 1270.66 | | 1282.61 | | 1288.85 | | 1300.59 | | 1322.94 | | 1325.88 | | 1327.89 | | 1338.38 | | 1342.81 | | 1361.71 | | 1379.92 | | 1386.85 | | 1394.53 | | 1516.80 | | 1522.56 | | 1524.52 | | 1528.25 | | 1543.74 | | 1555.35 | | 3058.13 | | 3058.38 | | 3070.84 | | 3077.74 | | 3079.80 | | 3081.53 | | 3102.49 | | 3107.58 | | 3110.68 | | 3115.24 | | 3121.68 | | 3128.76 | | 3133.07 | | 3142.69 | | 3147.66 | | 3153.78 | | |  | | --- | | 25.6421 | | 22.7448 | | 9.3207 | | 11.857 | | 6.2506 | | 0.0589 | | 14.9395 | | 0.0245 | | 0.0486 | | 12.709 | | 2.5148 | | 5.491 | | 0.2685 | | 346.0482 | | 6249.947 | | 1.2896 | | 0.3906 | | 1.5668 | | 1.2026 | | 0.877 | | 3.0285 | | 0.6862 | | 0.1211 | | 0.674 | | 0.3208 | | 1.3336 | | 2.0928 | | 2.7818 | | 0.5033 | | 3.768 | | 4.0835 | | 0.047 | | 2.1406 | | 2.9419 | | 0.1166 | | 0.5983 | | 0.0365 | | 0.1203 | | 5.4355 | | 0.006 | | 0.078 | | 16.7433 | | 4.1751 | | 0.1602 | | 2.1474 | | 0.5635 | | 0.239 | | 0.0271 | | 0.2164 | | 1.4072 | | 1.7581 | | 3.5069 | | 10.8286 | | 3.5039 | | 17.5979 | | 0.3925 | | 48.4038 | | 1.9854 | | 0.2317 | | 18.0932 | | 40.5805 | | 13.3299 | | 34.325 | | 56.1495 | | 22.4837 | | 68.6684 | | 53.9451 | | 62.6216 | | 83.2044 | | 80.5284 | | 6.5876 | | 53.4766 | | 2.3256 | | 85.9346 | | 53.095 | | 124.8937 | | 40.6011 | | 186.3386 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS1 JP-10/AlO** | | **TS2 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -993.18 | | ν2 | 15.07 | | ν3 | 37.91 | | ν4 | 68.90 | | ν5 | 94.27 | | ν6 | 141.69 | | ν7 | 180.78 | | ν8 | 260.90 | | ν9 | 315.90 | | ν10 | 332.00 | | ν11 | 389.81 | | ν12 | 495.85 | | ν13 | 537.64 | | ν14 | 557.48 | | ν15 | 667.08 | | ν16 | 734.33 | | ν17 | 752.02 | | ν18 | 768.47 | | ν19 | 809.94 | | ν20 | 842.54 | | ν21 | 880.79 | | ν22 | 882.56 | | ν23 | 912.87 | | ν24 | 920.62 | | ν25 | 934.72 | | ν26 | 941.74 | | ν27 | 951.71 | | ν28 | 976.70 | | ν29 | 986.48 | | ν30 | 1018.09 | | ν31 | 1034.54 | | ν32 | 1043.31 | | ν33 | 1067.46 | | ν34 | 1069.52 | | ν35 | 1076.25 | | ν36 | 1095.15 | | ν37 | 1115.83 | | ν38 | 1159.23 | | ν39 | 1167.65 | | ν40 | 1185.71 | | ν41 | 1213.93 | | ν42 | 1216.48 | | ν43 | 1236.12 | | ν44 | 1248.98 | | ν45 | 1267.63 | | ν46 | 1283.06 | | ν47 | 1290.68 | | ν48 | 1306.98 | | ν49 | 1315.01 | | ν50 | 1322.52 | | ν51 | 1331.50 | | ν52 | 1337.38 | | ν53 | 1353.80 | | ν54 | 1361.44 | | ν55 | 1363.28 | | ν56 | 1380.52 | | ν57 | 1387.71 | | ν58 | 1405.49 | | ν59 | 1522.55 | | ν60 | 1527.27 | | ν61 | 1529.11 | | ν62 | 1539.75 | | ν63 | 1554.97 | | ν64 | 3071.97 | | ν65 | 3075.29 | | ν66 | 3076.26 | | ν67 | 3076.47 | | ν68 | 3086.36 | | ν69 | 3087.78 | | ν70 | 3099.11 | | ν71 | 3107.87 | | ν72 | 3119.80 | | ν73 | 3125.77 | | ν74 | 3131.92 | | ν75 | 3136.69 | | ν76 | 3145.57 | | ν77 | 3146.67 | | ν78 | 3164.93 | | | |  | | --- | | 3271.0801 | | 0.6036 | | 1.3788 | | 1.9381 | | 1.5553 | | 1.8133 | | 1.6986 | | 7.1931 | | 4.5934 | | 0.3452 | | 6.4701 | | 0.5424 | | 0.6849 | | 2.8863 | | 2.3878 | | 215.7418 | | 0.4921 | | 4.2508 | | 15.2431 | | 48.3448 | | 3.8704 | | 0.6114 | | 3.1449 | | 9.0941 | | 5.702 | | 0.9562 | | 2.1183 | | 57.0062 | | 9.5641 | | 5.002 | | 1.8888 | | 173.9589 | | 9.9572 | | 3.8903 | | 6.9806 | | 335.7539 | | 306.2841 | | 54.201 | | 3.5998 | | 65.1352 | | 18.7186 | | 3.488 | | 51.9013 | | 1.2905 | | 350.9143 | | 1.4906 | | 47.9646 | | 63.6984 | | 112.9603 | | 0.5279 | | 9.9816 | | 19.2741 | | 242.3153 | | 12.7241 | | 27.5868 | | 7.8964 | | 36.7655 | | 88.9104 | | 2.2965 | | 4.6915 | | 7.2459 | | 7.4257 | | 12.9158 | | 11.5525 | | 14.0227 | | 27.7301 | | 22.6662 | | 10.6618 | | 49.102 | | 13.4361 | | 43.1271 | | 35.7314 | | 8.2309 | | 31.3563 | | 28.2931 | | 4.1161 | | 70.8167 | | 23.1997 | | |  | | --- | | -868.58 | | 31.73 | | 37.91 | | 133.74 | | 177.30 | | 259.29 | | 312.03 | | 327.23 | | 401.99 | | 454.51 | | 480.71 | | 497.70 | | 537.57 | | 548.80 | | 568.20 | | 668.08 | | 748.01 | | 764.82 | | 817.49 | | 843.58 | | 875.91 | | 879.48 | | 906.64 | | 914.69 | | 937.09 | | 939.45 | | 953.05 | | 977.54 | | 1002.14 | | 1020.42 | | 1027.08 | | 1049.87 | | 1063.05 | | 1072.76 | | 1080.74 | | 1091.84 | | 1127.60 | | 1146.34 | | 1168.83 | | 1202.68 | | 1213.82 | | 1217.38 | | 1233.93 | | 1250.61 | | 1265.50 | | 1280.44 | | 1288.33 | | 1303.73 | | 1308.87 | | 1320.04 | | 1325.09 | | 1332.27 | | 1347.50 | | 1360.21 | | 1363.69 | | 1382.08 | | 1390.27 | | 1522.28 | | 1522.80 | | 1527.11 | | 1532.43 | | 1546.16 | | 1559.27 | | 3072.42 | | 3072.56 | | 3074.06 | | 3079.45 | | 3085.48 | | 3088.45 | | 3091.45 | | 3094.45 | | 3110.04 | | 3127.94 | | 3131.41 | | 3136.60 | | 3146.72 | | 3152.27 | | 3160.96 | | |  | | --- | | 19417.4124 | | 0.2087 | | 0.5568 | | 0.041 | | 0.5322 | | 0.0381 | | 18.2947 | | 9.5249 | | 9.111 | | 360.8925 | | 1157.0138 | | 98.4125 | | 1038.8907 | | 68.351 | | 19.153 | | 11.068 | | 12.8386 | | 3.0538 | | 18.4656 | | 0.8002 | | 8.954 | | 0.8683 | | 4.5759 | | 25.4844 | | 9.5041 | | 2.303 | | 43.5399 | | 2.5348 | | 6.134 | | 27.0318 | | 6.9098 | | 297.9475 | | 13.122 | | 2.8982 | | 12.7665 | | 54.0248 | | 321.1419 | | 50.1873 | | 1.2847 | | 483.4916 | | 0.3349 | | 1.1 | | 37.4861 | | 474.2419 | | 255.1189 | | 36.6831 | | 684.0329 | | 1305.6723 | | 144.4434 | | 1.4243 | | 68.164 | | 13.162 | | 500.8126 | | 181.3874 | | 995.156 | | 143.2575 | | 1922.4873 | | 11.3465 | | 2.2441 | | 11.0037 | | 8.3384 | | 54.4113 | | 97.4121 | | 7.1476 | | 36.6055 | | 20.0482 | | 29.6881 | | 13.9053 | | 27.1617 | | 88.6767 | | 9.3349 | | 92.4328 | | 38.4383 | | 2.8344 | | 27.8708 | | 39.6767 | | 65.8554 | | 30.905 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS3** | | **TS4** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -1325.81 | | ν2 | 58.12 | | ν3 | 61.39 | | ν4 | 142.33 | | ν5 | 177.69 | | ν6 | 260.77 | | ν7 | 314.03 | | ν8 | 319.86 | | ν9 | 332.10 | | ν10 | 371.01 | | ν11 | 390.28 | | ν12 | 464.01 | | ν13 | 535.35 | | ν14 | 552.10 | | ν15 | 619.19 | | ν16 | 671.96 | | ν17 | 745.33 | | ν18 | 778.26 | | ν19 | 810.55 | | ν20 | 841.49 | | ν21 | 882.58 | | ν22 | 883.44 | | ν23 | 908.65 | | ν24 | 927.29 | | ν25 | 930.50 | | ν26 | 943.54 | | ν27 | 945.96 | | ν28 | 966.58 | | ν29 | 978.52 | | ν30 | 1019.48 | | ν31 | 1029.38 | | ν32 | 1059.41 | | ν33 | 1061.90 | | ν34 | 1071.01 | | ν35 | 1076.45 | | ν36 | 1095.94 | | ν37 | 1108.91 | | ν38 | 1117.51 | | ν39 | 1171.46 | | ν40 | 1186.92 | | ν41 | 1213.09 | | ν42 | 1223.95 | | ν43 | 1224.59 | | ν44 | 1229.33 | | ν45 | 1263.33 | | ν46 | 1267.52 | | ν47 | 1289.24 | | ν48 | 1295.07 | | ν49 | 1313.98 | | ν50 | 1320.17 | | ν51 | 1326.31 | | ν52 | 1341.82 | | ν53 | 1353.67 | | ν54 | 1364.21 | | ν55 | 1365.94 | | ν56 | 1389.90 | | ν57 | 1390.45 | | ν58 | 1510.95 | | ν59 | 1523.24 | | ν60 | 1528.10 | | ν61 | 1530.97 | | ν62 | 1545.45 | | ν63 | 1552.39 | | ν64 | 3066.91 | | ν65 | 3067.45 | | ν66 | 3077.66 | | ν67 | 3081.73 | | ν68 | 3087.42 | | ν69 | 3090.65 | | ν70 | 3092.87 | | ν71 | 3104.51 | | ν72 | 3120.35 | | ν73 | 3123.41 | | ν74 | 3124.54 | | ν75 | 3128.90 | | ν76 | 3148.05 | | ν77 | 3153.90 | | ν78 | 3158.81 | | | |  | | --- | | 28345.1992 | | 0.4065 | | 0.0571 | | 0.035 | | 1.3517 | | 0.0079 | | 0.035 | | 79.8031 | | 64.3034 | | 210.3668 | | 1.2096 | | 365.815 | | 0.9729 | | 39.291 | | 30.318 | | 0.0436 | | 0.267 | | 19.2688 | | 2.8624 | | 1.9319 | | 0.0161 | | 0.9171 | | 6.8158 | | 137.7507 | | 0.1477 | | 17.9595 | | 0.0018 | | 18.4975 | | 0.1233 | | 1.8017 | | 1.6633 | | 46.0838 | | 0.1181 | | 48.6169 | | 0.0508 | | 36.4342 | | 0.0179 | | 1251.742 | | 0.0845 | | 193.2214 | | 0.0099 | | 0.2758 | | 8.0293 | | 32.6305 | | 5.0074 | | 0.5716 | | 0.6485 | | 0.1574 | | 0.6872 | | 0.4244 | | 1.1007 | | 5.1984 | | 24.3743 | | 3.1226 | | 0.0549 | | 10.0203 | | 0.2554 | | 1494.6697 | | 2.4372 | | 2.0157 | | 361.8546 | | 1.8476 | | 405.8417 | | 2.8737 | | 37.3536 | | 26.2161 | | 33.3565 | | 117.1475 | | 58.8987 | | 24.4094 | | 47.56 | | 67.126 | | 20.9848 | | 31.8643 | | 3.928 | | 54.4735 | | 9.1335 | | 41.3255 | | |  | | --- | | -506.92 | | 34.97 | | 38.78 | | 127.23 | | 173.26 | | 258.67 | | 313.37 | | 326.16 | | 401.84 | | 488.58 | | 525.22 | | 552.02 | | 611.22 | | 686.53 | | 743.56 | | 765.90 | | 804.92 | | 834.89 | | 861.42 | | 875.21 | | 904.45 | | 917.89 | | 923.76 | | 937.05 | | 941.93 | | 952.86 | | 977.12 | | 981.78 | | 1016.95 | | 1031.01 | | 1056.85 | | 1067.63 | | 1074.80 | | 1092.43 | | 1133.45 | | 1159.03 | | 1174.91 | | 1196.76 | | 1202.03 | | 1213.40 | | 1229.39 | | 1254.46 | | 1269.86 | | 1272.80 | | 1282.69 | | 1289.33 | | 1303.18 | | 1321.43 | | 1324.52 | | 1327.40 | | 1331.81 | | 1345.92 | | 1360.32 | | 1383.78 | | 1384.72 | | 1416.71 | | 1516.89 | | 1522.43 | | 1528.22 | | 1532.79 | | 1545.77 | | 1557.89 | | 1652.19 | | 3056.45 | | 3069.70 | | 3076.86 | | 3077.93 | | 3082.03 | | 3082.44 | | 3089.83 | | 3109.58 | | 3118.97 | | 3127.31 | | 3130.74 | | 3134.39 | | 3141.98 | | 3147.84 | | 3167.72 | | |  | | --- | | 6870.1904 | | 0.4676 | | 0.3244 | | 0.1551 | | 17.1732 | | 3.0391 | | 1.6464 | | 23.4841 | | 0.4423 | | 141.9445 | | 8.6434 | | 28.4791 | | 2719.5648 | | 705.7731 | | 213.5919 | | 116.3752 | | 89.2432 | | 146.2567 | | 116.6038 | | 136.7934 | | 145.5968 | | 8.2154 | | 194.2148 | | 155.6536 | | 97.292 | | 370.8626 | | 78.0726 | | 9.2994 | | 268.8318 | | 143.5648 | | 77.6382 | | 25.842 | | 6.3745 | | 44.6204 | | 186.6093 | | 47.637 | | 269.8673 | | 334.0389 | | 462.5264 | | 243.8459 | | 455.6074 | | 765.7997 | | 50.4677 | | 271.2435 | | 191.0414 | | 50.8383 | | 1451.1853 | | 209.7029 | | 235.7564 | | 370.3159 | | 356.4206 | | 321.2419 | | 8.1924 | | 994.652 | | 1190.3273 | | 3487.3534 | | 21.0592 | | 10.2418 | | 209.784 | | 137.8874 | | 584.9517 | | 531.1511 | | 15293.0443 | | 42.7945 | | 30.2766 | | 65.7653 | | 44.8423 | | 55.2483 | | 5.0722 | | 118.7236 | | 101.34 | | 101.964 | | 28.5861 | | 37.9382 | | 62.2284 | | 107.5308 | | 39.9404 | | 164.6999 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS5** | | **TS6** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -1158.72 | | ν2 | 17.75 | | ν3 | 45.37 | | ν4 | 67.38 | | ν5 | 97.74 | | ν6 | 140.30 | | ν7 | 179.42 | | ν8 | 257.15 | | ν9 | 321.59 | | ν10 | 326.20 | | ν11 | 401.94 | | ν12 | 490.26 | | ν13 | 526.47 | | ν14 | 550.95 | | ν15 | 660.26 | | ν16 | 735.92 | | ν17 | 751.56 | | ν18 | 768.00 | | ν19 | 811.36 | | ν20 | 832.17 | | ν21 | 847.06 | | ν22 | 878.59 | | ν23 | 883.44 | | ν24 | 918.41 | | ν25 | 919.92 | | ν26 | 940.15 | | ν27 | 952.95 | | ν28 | 968.12 | | ν29 | 985.67 | | ν30 | 992.31 | | ν31 | 1021.84 | | ν32 | 1035.98 | | ν33 | 1063.30 | | ν34 | 1071.03 | | ν35 | 1075.45 | | ν36 | 1094.82 | | ν37 | 1129.45 | | ν38 | 1151.19 | | ν39 | 1163.34 | | ν40 | 1184.57 | | ν41 | 1217.07 | | ν42 | 1217.99 | | ν43 | 1233.35 | | ν44 | 1245.15 | | ν45 | 1269.51 | | ν46 | 1282.23 | | ν47 | 1291.12 | | ν48 | 1299.12 | | ν49 | 1312.12 | | ν50 | 1323.35 | | ν51 | 1332.99 | | ν52 | 1339.45 | | ν53 | 1341.81 | | ν54 | 1356.44 | | ν55 | 1359.17 | | ν56 | 1381.46 | | ν57 | 1389.95 | | ν58 | 1421.58 | | ν59 | 1523.57 | | ν60 | 1525.84 | | ν61 | 1532.88 | | ν62 | 1541.35 | | ν63 | 1556.09 | | ν64 | 3077.01 | | ν65 | 3080.35 | | ν66 | 3081.87 | | ν67 | 3087.42 | | ν68 | 3088.19 | | ν69 | 3090.47 | | ν70 | 3093.93 | | ν71 | 3102.29 | | ν72 | 3107.65 | | ν73 | 3117.76 | | ν74 | 3132.38 | | ν75 | 3137.45 | | ν76 | 3149.91 | | ν77 | 3152.17 | | ν78 | 3156.09 | | | |  | | --- | | 3759.1881 | | 0.9297 | | 1.0388 | | 1.9308 | | 1.4812 | | 1.8842 | | 0.2945 | | 3.5586 | | 4.6389 | | 2.5158 | | 0.6938 | | 5.8516 | | 5.7613 | | 13.3442 | | 35.5498 | | 211.9555 | | 0.2469 | | 0.3473 | | 4.7742 | | 322.8392 | | 82.6983 | | 0.6895 | | 2.9533 | | 0.2124 | | 8.5765 | | 0.1357 | | 1.4584 | | 26.2915 | | 3.6016 | | 46.4635 | | 3.174 | | 24.3536 | | 0.1935 | | 6.953 | | 0.2809 | | 1.3242 | | 101.804 | | 0.0461 | | 0.6913 | | 3.5788 | | 13.4337 | | 24.7971 | | 115.0117 | | 29.3118 | | 1.6024 | | 118.0556 | | 2.1482 | | 18.8512 | | 3.3056 | | 1.3616 | | 5.1105 | | 3.8294 | | 13.0719 | | 29.6278 | | 3.9005 | | 18.7961 | | 33.3653 | | 232.3392 | | 1.2818 | | 1.6271 | | 10.0424 | | 15.2491 | | 3.4104 | | 20.9239 | | 2.2236 | | 14.051 | | 38.9896 | | 10.7391 | | 64.2169 | | 11.9225 | | 60.8173 | | 22.1968 | | 29.3077 | | 0.1737 | | 34.1107 | | 8.2963 | | 56.63 | | 40.3093 | | |  | | --- | | -946.56 | | 33.83 | | 35.14 | | 41.11 | | 160.11 | | 251.06 | | 258.11 | | 320.24 | | 382.37 | | 477.83 | | 490.96 | | 573.23 | | 589.75 | | 603.77 | | 741.03 | | 742.19 | | 761.29 | | 790.15 | | 816.97 | | 823.60 | | 855.76 | | 881.92 | | 912.19 | | 919.06 | | 943.78 | | 945.61 | | 955.82 | | 982.59 | | 985.20 | | 1013.11 | | 1043.75 | | 1053.64 | | 1061.95 | | 1086.36 | | 1100.78 | | 1121.16 | | 1135.16 | | 1156.62 | | 1165.20 | | 1179.99 | | 1218.11 | | 1227.11 | | 1239.78 | | 1267.91 | | 1291.99 | | 1293.15 | | 1303.38 | | 1305.58 | | 1309.69 | | 1325.97 | | 1334.26 | | 1335.36 | | 1352.02 | | 1360.78 | | 1369.12 | | 1387.20 | | 1402.36 | | 1426.48 | | 1515.59 | | 1525.58 | | 1530.59 | | 1534.69 | | 1555.94 | | 3070.22 | | 3073.96 | | 3077.92 | | 3081.33 | | 3087.06 | | 3087.71 | | 3093.33 | | 3111.24 | | 3113.71 | | 3117.16 | | 3128.24 | | 3130.82 | | 3139.01 | | 3147.99 | | 3172.80 | | |  | | --- | | 18912.2857 | | 0.497 | | 0.5439 | | 0.0512 | | 20.6319 | | 0.0274 | | 3.6134 | | 0.5154 | | 107.5092 | | 47.0846 | | 2.7515 | | 665.8624 | | 152.6882 | | 744.5175 | | 26.4033 | | 472.618 | | 36.3075 | | 0.5968 | | 7.1642 | | 11.9444 | | 1.5017 | | 25.407 | | 13.8276 | | 1.6695 | | 18.9403 | | 3.1107 | | 3.5664 | | 22.8298 | | 0.007 | | 24.8285 | | 11.5583 | | 3.7777 | | 32.5282 | | 37.6049 | | 39.3276 | | 7.4585 | | 5.1841 | | 0.0105 | | 4.6154 | | 0.0629 | | 23.0516 | | 0.2106 | | 40.6947 | | 0.3671 | | 0.4979 | | 839.8128 | | 8.6148 | | 0.7029 | | 0.1947 | | 0.3836 | | 2.895 | | 934.7217 | | 7.4466 | | 3073.7504 | | 642.2788 | | 2.7069 | | 3829.5869 | | 304.7077 | | 8.1047 | | 2.1125 | | 68.5448 | | 50.0592 | | 5.8715 | | 9.4759 | | 5.8631 | | 8.5322 | | 62.4011 | | 25.0069 | | 62.9136 | | 49.8249 | | 84.109 | | 35.0188 | | 13.3744 | | 0.6156 | | 17.222 | | 62.7915 | | 71.3039 | | 35.7949 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 1 JP-10/AlO** | | **vdW2 Site 2 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 14.50 | | ν2 | 28.71 | | ν3 | 49.16 | | ν4 | 83.98 | | ν5 | 85.82 | | ν6 | 154.52 | | ν7 | 184.93 | | ν8 | 290.84 | | ν9 | 322.30 | | ν10 | 330.75 | | ν11 | 396.64 | | ν12 | 424.80 | | ν13 | 496.67 | | ν14 | 528.13 | | ν15 | 554.88 | | ν16 | 569.01 | | ν17 | 622.78 | | ν18 | 668.61 | | ν19 | 758.30 | | ν20 | 781.20 | | ν21 | 815.48 | | ν22 | 868.05 | | ν23 | 880.24 | | ν24 | 884.61 | | ν25 | 915.25 | | ν26 | 924.00 | | ν27 | 930.17 | | ν28 | 941.10 | | ν29 | 956.53 | | ν30 | 961.14 | | ν31 | 987.50 | | ν32 | 1009.52 | | ν33 | 1024.89 | | ν34 | 1037.24 | | ν35 | 1057.01 | | ν36 | 1064.25 | | ν37 | 1075.33 | | ν38 | 1100.11 | | ν39 | 1151.06 | | ν40 | 1166.71 | | ν41 | 1173.91 | | ν42 | 1201.97 | | ν43 | 1215.99 | | ν44 | 1231.72 | | ν45 | 1254.69 | | ν46 | 1271.92 | | ν47 | 1286.45 | | ν48 | 1297.24 | | ν49 | 1306.27 | | ν50 | 1319.37 | | ν51 | 1333.04 | | ν52 | 1342.42 | | ν53 | 1350.73 | | ν54 | 1357.90 | | ν55 | 1362.69 | | ν56 | 1376.50 | | ν57 | 1385.56 | | ν58 | 1512.03 | | ν59 | 1526.18 | | ν60 | 1527.78 | | ν61 | 1539.68 | | ν62 | 1558.13 | | ν63 | 3046.46 | | ν64 | 3075.35 | | ν65 | 3076.08 | | ν66 | 3076.69 | | ν67 | 3077.81 | | ν68 | 3092.47 | | ν69 | 3101.12 | | ν70 | 3107.42 | | ν71 | 3121.45 | | ν72 | 3126.28 | | ν73 | 3131.48 | | ν74 | 3137.17 | | ν75 | 3146.43 | | ν76 | 3171.04 | | ν77 | 3211.00 | | ν78 | 3829.35 | | | |  | | --- | | 0.4438 | | 0.8293 | | 3.3197 | | 1.9209 | | 1.0702 | | 1.3146 | | 1.2473 | | 2.282 | | 2.3938 | | 2.7654 | | 6.5069 | | 124.8752 | | 16.3606 | | 8.077 | | 9.1029 | | 253.0468 | | 96.6667 | | 0.6924 | | 2.1696 | | 0.8691 | | 2.1641 | | 119.8005 | | 0.3171 | | 2.1525 | | 0.326 | | 0.8407 | | 1.5938 | | 1.0605 | | 0.0937 | | 0.1039 | | 4.7214 | | 0.8099 | | 1.5222 | | 4.6087 | | 0.5526 | | 0.187 | | 0.1719 | | 0.8551 | | 1.1643 | | 0.0904 | | 0.7617 | | 0.9991 | | 0.2165 | | 0.5295 | | 2.7897 | | 0.6198 | | 1.1441 | | 1.8561 | | 0.773 | | 0.3827 | | 1.3297 | | 1.6305 | | 3.4632 | | 0.9821 | | 0.7806 | | 2.1353 | | 0.649 | | 6.6184 | | 5.6075 | | 3.854 | | 3.5376 | | 10.7005 | | 22.4845 | | 24.7163 | | 35.0363 | | 7.8626 | | 14.683 | | 26.5145 | | 26.7645 | | 13.62 | | 50.8805 | | 7.2878 | | 30.7653 | | 27.5649 | | 58.3402 | | 16.2888 | | 19.8519 | | 517.3454 | | |  | | --- | | 15.38 | | 30.35 | | 57.26 | | 70.31 | | 84.81 | | 137.52 | | 177.97 | | 263.57 | | 316.96 | | 328.94 | | 401.78 | | 412.58 | | 495.54 | | 519.82 | | 555.03 | | 561.28 | | 661.10 | | 731.21 | | 763.79 | | 801.70 | | 838.84 | | 857.77 | | 871.12 | | 878.19 | | 898.92 | | 914.57 | | 934.53 | | 940.05 | | 957.74 | | 974.92 | | 996.88 | | 1023.12 | | 1026.67 | | 1062.49 | | 1071.01 | | 1081.09 | | 1107.81 | | 1129.71 | | 1159.70 | | 1183.79 | | 1212.72 | | 1215.97 | | 1226.14 | | 1238.31 | | 1252.58 | | 1275.87 | | 1283.84 | | 1301.97 | | 1316.49 | | 1323.40 | | 1328.25 | | 1334.95 | | 1349.90 | | 1363.93 | | 1376.49 | | 1392.87 | | 1520.62 | | 1522.90 | | 1530.26 | | 1532.74 | | 1545.70 | | 1557.71 | | 3075.83 | | 3077.02 | | 3080.06 | | 3085.35 | | 3094.95 | | 3096.36 | | 3099.06 | | 3106.29 | | 3115.21 | | 3132.83 | | 3140.55 | | 3141.23 | | 3154.67 | | 3161.17 | | 3182.03 | | 3832.03 | | |  | | --- | | 0.5811 | | 0.8934 | | 2.8778 | | 1.9007 | | 0.2598 | | 0.3932 | | 0.3268 | | 0.6714 | | 0.1404 | | 0.511 | | 7.1358 | | 130.1957 | | 3.2553 | | 7.1771 | | 3.8743 | | 304.9999 | | 1.1614 | | 0.2935 | | 0.5796 | | 1.2223 | | 0.5841 | | 25.1437 | | 98.9828 | | 0.3358 | | 0.2642 | | 0.4327 | | 0.0898 | | 1.6672 | | 1.1416 | | 1.34 | | 0.4599 | | 0.873 | | 2.5587 | | 0.2051 | | 0.0475 | | 0.3044 | | 0.2303 | | 0.1352 | | 1.3217 | | 1.1865 | | 0.388 | | 0.6502 | | 6.017 | | 2.0005 | | 3.5195 | | 0.674 | | 0.8316 | | 3.7351 | | 2.1636 | | 2.5604 | | 1.8784 | | 2.9426 | | 0.9687 | | 0.3006 | | 0.4667 | | 0.485 | | 2.4956 | | 0.4724 | | 5.6419 | | 11.4116 | | 11.3645 | | 13.9771 | | 34.0972 | | 20.7292 | | 4.5443 | | 26.8912 | | 17.2787 | | 29.7478 | | 48.5599 | | 24.7099 | | 29.8274 | | 25.8844 | | 6.485 | | 28.2929 | | 28.8077 | | 45.1915 | | 16.8376 | | 497.0561 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 3 JP-10/AlO** | | **vdW2 Site 4 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 22.85 | | ν2 | 33.25 | | ν3 | 46.46 | | ν4 | 69.91 | | ν5 | 102.74 | | ν6 | 125.39 | | ν7 | 187.28 | | ν8 | 247.52 | | ν9 | 315.56 | | ν10 | 328.22 | | ν11 | 379.10 | | ν12 | 380.25 | | ν13 | 456.06 | | ν14 | 531.35 | | ν15 | 542.38 | | ν16 | 557.50 | | ν17 | 667.49 | | ν18 | 743.84 | | ν19 | 766.56 | | ν20 | 798.42 | | ν21 | 808.77 | | ν22 | 852.01 | | ν23 | 863.64 | | ν24 | 876.69 | | ν25 | 887.46 | | ν26 | 904.89 | | ν27 | 931.95 | | ν28 | 944.01 | | ν29 | 947.14 | | ν30 | 971.67 | | ν31 | 976.20 | | ν32 | 1018.72 | | ν33 | 1024.01 | | ν34 | 1040.51 | | ν35 | 1066.45 | | ν36 | 1071.32 | | ν37 | 1076.39 | | ν38 | 1096.56 | | ν39 | 1173.41 | | ν40 | 1182.74 | | ν41 | 1209.69 | | ν42 | 1214.39 | | ν43 | 1223.91 | | ν44 | 1224.67 | | ν45 | 1248.19 | | ν46 | 1263.42 | | ν47 | 1286.20 | | ν48 | 1286.27 | | ν49 | 1311.62 | | ν50 | 1319.62 | | ν51 | 1325.03 | | ν52 | 1344.46 | | ν53 | 1348.80 | | ν54 | 1363.58 | | ν55 | 1363.71 | | ν56 | 1381.53 | | ν57 | 1383.07 | | ν58 | 1523.06 | | ν59 | 1526.38 | | ν60 | 1527.50 | | ν61 | 1543.66 | | ν62 | 1545.74 | | ν63 | 3073.80 | | ν64 | 3076.71 | | ν65 | 3081.95 | | ν66 | 3086.41 | | ν67 | 3087.25 | | ν68 | 3090.17 | | ν69 | 3092.91 | | ν70 | 3129.99 | | ν71 | 3131.90 | | ν72 | 3135.50 | | ν73 | 3136.40 | | ν74 | 3144.15 | | ν75 | 3150.64 | | ν76 | 3153.14 | | ν77 | 3190.45 | | ν78 | 3861.54 | | | |  | | --- | | 1.8074 | | 0.0127 | | 3.9092 | | 0.8148 | | 1.8402 | | 0.8564 | | 0.814 | | 0.1899 | | 2.7301 | | 2.1775 | | 10.2494 | | 119.7963 | | 32.0656 | | 1.635 | | 55.5414 | | 98.4691 | | 0.0016 | | 1.2305 | | 14.2776 | | 7.9257 | | 3.3219 | | 0.5198 | | 145.0037 | | 0.7453 | | 0.1637 | | 0.2699 | | 0.1096 | | 2.3859 | | 0.3047 | | 0.9748 | | 2.6045 | | 1.6824 | | 1.3765 | | 0.1201 | | 0.1816 | | 0.091 | | 0.1953 | | 0.8159 | | 1.6252 | | 1.8898 | | 0.5277 | | 0.1922 | | 0.2955 | | 1.5325 | | 1.4233 | | 0.2341 | | 4.2162 | | 0.1945 | | 0.0067 | | 0.0397 | | 0.5484 | | 3.2325 | | 0.3153 | | 0.5017 | | 0.3836 | | 4.4837 | | 0.1273 | | 3.1338 | | 2.0034 | | 10.3457 | | 2.0939 | | 4.5482 | | 31.4969 | | 1.4939 | | 27.2288 | | 36.4234 | | 8.228 | | 19.6697 | | 71.3293 | | 22.0899 | | 23.2237 | | 0.1993 | | 27.1875 | | 19.6173 | | 36.6547 | | 60.144 | | 18.3199 | | 448.7079 | | |  | | --- | | 16.04 | | 22.06 | | 45.13 | | 72.23 | | 88.61 | | 117.39 | | 174.33 | | 244.51 | | 301.12 | | 317.06 | | 392.56 | | 469.83 | | 487.09 | | 540.73 | | 555.07 | | 558.18 | | 635.65 | | 730.36 | | 754.47 | | 812.02 | | 839.79 | | 865.76 | | 869.70 | | 896.49 | | 902.36 | | 916.33 | | 921.16 | | 933.76 | | 947.07 | | 981.38 | | 983.65 | | 1021.22 | | 1037.30 | | 1062.02 | | 1070.71 | | 1080.00 | | 1113.06 | | 1145.48 | | 1148.18 | | 1174.32 | | 1179.61 | | 1208.67 | | 1231.02 | | 1246.74 | | 1250.11 | | 1268.40 | | 1277.97 | | 1289.96 | | 1322.42 | | 1323.50 | | 1331.22 | | 1334.70 | | 1356.47 | | 1359.16 | | 1370.10 | | 1384.60 | | 1505.93 | | 1521.49 | | 1526.15 | | 1531.38 | | 1541.15 | | 1555.98 | | 3026.47 | | 3057.94 | | 3075.76 | | 3082.39 | | 3083.37 | | 3085.98 | | 3096.50 | | 3100.11 | | 3120.90 | | 3131.79 | | 3137.84 | | 3143.55 | | 3145.92 | | 3151.02 | | 3166.33 | | 3769.73 | | |  | | --- | | 0.2555 | | 1.6762 | | 3.1994 | | 0.8824 | | 0.4484 | | 0.4828 | | 1.6412 | | 3.1036 | | 0.3371 | | 1.6639 | | 0.3735 | | 130.4129 | | 1.2211 | | 4.3416 | | 58.2908 | | 172.239 | | 12.5175 | | 0.3412 | | 0.648 | | 1.99 | | 6.8955 | | 0.2884 | | 120.5194 | | 1.9442 | | 0.2877 | | 0.7775 | | 0.4257 | | 0.3464 | | 1.2835 | | 2.3953 | | 2.0246 | | 1.7741 | | 1.8759 | | 0.6446 | | 0.1404 | | 0.0795 | | 1.9771 | | 0.4244 | | 0.3583 | | 0.2448 | | 0.7034 | | 1.5663 | | 1.1657 | | 2.7825 | | 0.0977 | | 0.0664 | | 0.7467 | | 0.9533 | | 0.0945 | | 0.3995 | | 3.8402 | | 4.2951 | | 1.2905 | | 0.2039 | | 0.7192 | | 0.9923 | | 7.1635 | | 1.447 | | 2.907 | | 6.653 | | 12.3028 | | 6.0946 | | 25.0339 | | 9.8296 | | 12.5853 | | 42.2395 | | 16.7104 | | 19.6542 | | 46.1853 | | 27.3039 | | 48.5908 | | 26.0739 | | 34.3841 | | 9.1872 | | 11.305 | | 46.3075 | | 29.4946 | | 596.8993 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 5 JP-10/AlO** | | **vdW2 Site 6 JP-10/AlO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 7.05 | | ν2 | 12.61 | | ν3 | 40.89 | | ν4 | 62.69 | | ν5 | 91.22 | | ν6 | 124.63 | | ν7 | 138.93 | | ν8 | 256.01 | | ν9 | 281.12 | | ν10 | 313.28 | | ν11 | 352.42 | | ν12 | 380.08 | | ν13 | 403.87 | | ν14 | 473.62 | | ν15 | 499.38 | | ν16 | 535.94 | | ν17 | 632.14 | | ν18 | 745.68 | | ν19 | 761.27 | | ν20 | 770.52 | | ν21 | 814.37 | | ν22 | 847.23 | | ν23 | 852.93 | | ν24 | 862.90 | | ν25 | 887.86 | | ν26 | 918.55 | | ν27 | 936.22 | | ν28 | 950.26 | | ν29 | 954.36 | | ν30 | 976.92 | | ν31 | 985.95 | | ν32 | 1003.82 | | ν33 | 1033.40 | | ν34 | 1043.02 | | ν35 | 1065.10 | | ν36 | 1073.54 | | ν37 | 1097.50 | | ν38 | 1103.43 | | ν39 | 1138.74 | | ν40 | 1156.37 | | ν41 | 1178.40 | | ν42 | 1207.46 | | ν43 | 1228.57 | | ν44 | 1239.91 | | ν45 | 1257.03 | | ν46 | 1265.21 | | ν47 | 1291.15 | | ν48 | 1297.77 | | ν49 | 1316.07 | | ν50 | 1321.02 | | ν51 | 1329.95 | | ν52 | 1333.38 | | ν53 | 1339.26 | | ν54 | 1348.33 | | ν55 | 1370.14 | | ν56 | 1378.01 | | ν57 | 1389.45 | | ν58 | 1515.07 | | ν59 | 1524.86 | | ν60 | 1527.77 | | ν61 | 1544.22 | | ν62 | 1555.19 | | ν63 | 3030.04 | | ν64 | 3033.47 | | ν65 | 3080.00 | | ν66 | 3084.28 | | ν67 | 3088.74 | | ν68 | 3089.61 | | ν69 | 3096.84 | | ν70 | 3103.82 | | ν71 | 3115.15 | | ν72 | 3122.76 | | ν73 | 3130.20 | | ν74 | 3144.36 | | ν75 | 3149.58 | | ν76 | 3151.52 | | ν77 | 3221.03 | | ν78 | 3914.16 | | | |  | | --- | | 0.1182 | | 0.7093 | | 1.009 | | 3.9369 | | 2.3488 | | 1.1393 | | 8.6535 | | 1.9826 | | 3.9451 | | 3.3422 | | 32.5757 | | 267.2557 | | 22.5437 | | 187.9611 | | 1.0409 | | 0.2863 | | 3.6395 | | 0.5377 | | 3.7474 | | 0.0051 | | 0.7192 | | 2.1336 | | 2.5354 | | 126.4786 | | 2.0407 | | 0.5427 | | 0.216 | | 0.1624 | | 1.6827 | | 2.3123 | | 0.4987 | | 1.8962 | | 0.7936 | | 0.6496 | | 0.434 | | 0.0109 | | 0.4465 | | 1.3938 | | 0.1942 | | 0.1821 | | 0.755 | | 0.2862 | | 5.1441 | | 1.5266 | | 0.1804 | | 0.2436 | | 2.0579 | | 0.3451 | | 0.7717 | | 0.3035 | | 0.0949 | | 2.9746 | | 1.8571 | | 5.2465 | | 2.8716 | | 2.6491 | | 1.3475 | | 3.0322 | | 2.3341 | | 4.161 | | 18.26 | | 4.6603 | | 23.2447 | | 23.8624 | | 21.2361 | | 15.3115 | | 24.6959 | | 50.3149 | | 28.1373 | | 21.7177 | | 66.3084 | | 15.4141 | | 0.8461 | | 24.4747 | | 64.4202 | | 23.5965 | | 16.5974 | | 288.6037 | | |  | | --- | | 14.12 | | 29.20 | | 45.26 | | 71.45 | | 87.38 | | 120.09 | | 160.36 | | 253.09 | | 284.85 | | 323.98 | | 402.37 | | 434.58 | | 461.85 | | 500.46 | | 532.69 | | 552.99 | | 697.28 | | 700.59 | | 745.98 | | 789.42 | | 811.09 | | 841.62 | | 862.77 | | 868.93 | | 913.56 | | 920.64 | | 935.57 | | 949.61 | | 952.36 | | 971.79 | | 986.96 | | 991.87 | | 1037.56 | | 1055.06 | | 1066.84 | | 1075.82 | | 1087.08 | | 1097.67 | | 1149.63 | | 1161.60 | | 1170.80 | | 1206.34 | | 1218.74 | | 1232.37 | | 1255.38 | | 1267.33 | | 1286.12 | | 1295.75 | | 1311.84 | | 1325.38 | | 1329.58 | | 1334.84 | | 1336.09 | | 1363.45 | | 1368.27 | | 1381.68 | | 1393.33 | | 1506.54 | | 1509.58 | | 1525.17 | | 1534.94 | | 1554.91 | | 3004.88 | | 3005.98 | | 3080.04 | | 3082.58 | | 3089.58 | | 3090.11 | | 3090.59 | | 3109.37 | | 3112.93 | | 3115.61 | | 3123.94 | | 3131.04 | | 3142.61 | | 3150.57 | | 3213.20 | | 3834.67 | | |  | | --- | | 0.758 | | 0.2424 | | 3.5525 | | 0.1727 | | 1.577 | | 0.2363 | | 5.7919 | | 0.5596 | | 1.9617 | | 2.7344 | | 1.9801 | | 119.7852 | | 20.7013 | | 20.1988 | | 0.0356 | | 316.9114 | | 0.9507 | | 4.4179 | | 0.431 | | 0.3052 | | 0.8662 | | 2.0316 | | 1.0313 | | 120.7525 | | 1.8624 | | 0.3778 | | 0.9232 | | 0.3984 | | 1.6662 | | 1.3146 | | 0.548 | | 2.2688 | | 3.0623 | | 0.2724 | | 0.5769 | | 0.1256 | | 0.0537 | | 0.0329 | | 0.7467 | | 0.0346 | | 0.7427 | | 0.1685 | | 0.029 | | 3.6319 | | 2.7196 | | 0.1171 | | 1.1349 | | 0.3102 | | 0.117 | | 0.0274 | | 0.464 | | 5.9386 | | 0.3018 | | 0.3423 | | 7.5949 | | 0.6564 | | 0.655 | | 10.5987 | | 4.2552 | | 1.6738 | | 18.8879 | | 5.6066 | | 21.4429 | | 22.6578 | | 19.5436 | | 23.397 | | 58.3059 | | 11.5354 | | 8.3503 | | 2.6276 | | 82.4087 | | 29.4235 | | 14.701 | | 0.0045 | | 27.2062 | | 60.97 | | 25.9556 | | 430.6408 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 1 JP-10/BO** | | **vdW1 Site2 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 25.22 | | ν2 | 28.20 | | ν3 | 41.87 | | ν4 | 47.01 | | ν5 | 64.05 | | ν6 | 135.43 | | ν7 | 179.85 | | ν8 | 261.57 | | ν9 | 318.68 | | ν10 | 332.36 | | ν11 | 404.33 | | ν12 | 496.04 | | ν13 | 533.01 | | ν14 | 556.37 | | ν15 | 668.85 | | ν16 | 752.97 | | ν17 | 766.82 | | ν18 | 811.44 | | ν19 | 843.38 | | ν20 | 881.79 | | ν21 | 883.10 | | ν22 | 916.33 | | ν23 | 918.54 | | ν24 | 941.19 | | ν25 | 942.64 | | ν26 | 952.36 | | ν27 | 985.14 | | ν28 | 985.59 | | ν29 | 1020.62 | | ν30 | 1028.53 | | ν31 | 1066.23 | | ν32 | 1069.03 | | ν33 | 1075.24 | | ν34 | 1076.52 | | ν35 | 1095.19 | | ν36 | 1155.16 | | ν37 | 1170.51 | | ν38 | 1183.65 | | ν39 | 1215.19 | | ν40 | 1221.52 | | ν41 | 1227.43 | | ν42 | 1245.21 | | ν43 | 1270.57 | | ν44 | 1287.39 | | ν45 | 1294.04 | | ν46 | 1307.14 | | ν47 | 1319.85 | | ν48 | 1326.67 | | ν49 | 1334.36 | | ν50 | 1342.10 | | ν51 | 1345.50 | | ν52 | 1363.09 | | ν53 | 1364.93 | | ν54 | 1384.20 | | ν55 | 1387.91 | | ν56 | 1522.93 | | ν57 | 1524.98 | | ν58 | 1529.17 | | ν59 | 1533.93 | | ν60 | 1547.80 | | ν61 | 1561.58 | | ν62 | 1912.39 | | ν63 | 3067.19 | | ν64 | 3070.54 | | ν65 | 3076.32 | | ν66 | 3081.66 | | ν67 | 3083.60 | | ν68 | 3083.90 | | ν69 | 3086.32 | | ν70 | 3087.53 | | ν71 | 3109.53 | | ν72 | 3115.32 | | ν73 | 3126.21 | | ν74 | 3129.36 | | ν75 | 3139.90 | | ν76 | 3145.71 | | ν77 | 3147.62 | | ν78 | 3165.12 | | | |  | | --- | | 10.2391 | | 11.4026 | | 8.1567 | | 6.1212 | | 0.3342 | | 0.0037 | | 0.0551 | | 0.0464 | | 0.0704 | | 0.4163 | | 0.0015 | | 0.4426 | | 0.2006 | | 1.5602 | | 0.83 | | 0.3057 | | 0.7247 | | 0.9058 | | 0.8878 | | 1.0874 | | 2.134 | | 0.0836 | | 0.9404 | | 0.082 | | 1.5478 | | 1.4747 | | 2.321 | | 0.3338 | | 2.0434 | | 1.4684 | | 0.0209 | | 0.2564 | | 0.0453 | | 0.0612 | | 0.8207 | | 0.1692 | | 0.2051 | | 1.6119 | | 0.1902 | | 0.0875 | | 2.3231 | | 1.3384 | | 0.022 | | 3.0543 | | 0.772 | | 0.0025 | | 0.0501 | | 0.3669 | | 0.2285 | | 5.7713 | | 0.0122 | | 0.283 | | 2.1026 | | 3.3768 | | 0.1504 | | 1.3486 | | 2.6419 | | 2.8968 | | 8.6982 | | 9.8715 | | 5.5372 | | 143.8264 | | 3.1441 | | 37.068 | | 23.1088 | | 31.672 | | 45.5786 | | 28.7317 | | 69.1679 | | 3.5902 | | 87.9166 | | 10.3538 | | 0.2346 | | 28.9422 | | 20.663 | | 15.8866 | | 99.8338 | | 11.9748 | | |  | | --- | | 24.97 | | 27.95 | | 41.75 | | 46.93 | | 64.06 | | 135.44 | | 179.85 | | 261.57 | | 318.68 | | 332.36 | | 404.34 | | 496.04 | | 533.01 | | 556.37 | | 668.85 | | 752.97 | | 766.82 | | 811.43 | | 843.38 | | 881.79 | | 883.11 | | 916.33 | | 918.54 | | 941.19 | | 942.64 | | 952.34 | | 985.15 | | 985.58 | | 1020.62 | | 1028.53 | | 1066.24 | | 1069.03 | | 1075.24 | | 1076.53 | | 1095.19 | | 1155.16 | | 1170.51 | | 1183.65 | | 1215.19 | | 1221.52 | | 1227.43 | | 1245.21 | | 1270.57 | | 1287.39 | | 1294.04 | | 1307.14 | | 1319.85 | | 1326.67 | | 1334.36 | | 1342.10 | | 1345.50 | | 1363.09 | | 1364.93 | | 1384.20 | | 1387.91 | | 1522.93 | | 1524.98 | | 1529.17 | | 1533.93 | | 1547.80 | | 1561.58 | | 1912.43 | | 3067.19 | | 3070.54 | | 3076.32 | | 3081.66 | | 3083.60 | | 3083.90 | | 3086.32 | | 3087.53 | | 3109.53 | | 3115.31 | | 3126.21 | | 3129.35 | | 3139.90 | | 3145.71 | | 3147.62 | | 3165.12 | | |  | | --- | | 10.4206 | | 11.5301 | | 7.9755 | | 5.9934 | | 0.3339 | | 0.0037 | | 0.0551 | | 0.0464 | | 0.0704 | | 0.4164 | | 0.0015 | | 0.4426 | | 0.2006 | | 1.5603 | | 0.8301 | | 0.3057 | | 0.7247 | | 0.906 | | 0.8877 | | 1.0875 | | 2.134 | | 0.0836 | | 0.9408 | | 0.082 | | 1.5473 | | 1.4751 | | 2.3208 | | 0.3341 | | 2.043 | | 1.4685 | | 0.0209 | | 0.2564 | | 0.0453 | | 0.0612 | | 0.8207 | | 0.1692 | | 0.205 | | 1.6117 | | 0.1901 | | 0.0876 | | 2.3231 | | 1.3386 | | 0.0219 | | 3.055 | | 0.7725 | | 0.0024 | | 0.0501 | | 0.3669 | | 0.2295 | | 5.7694 | | 0.0122 | | 0.283 | | 2.1027 | | 3.3774 | | 0.1504 | | 1.3468 | | 2.6413 | | 2.8972 | | 8.7018 | | 9.8705 | | 5.5366 | | 143.8168 | | 3.1412 | | 37.0687 | | 23.1088 | | 31.6419 | | 45.5826 | | 28.7855 | | 69.1636 | | 3.5741 | | 87.9197 | | 10.3542 | | 0.2332 | | 28.9439 | | 20.6566 | | 15.8678 | | 99.8489 | | 11.9752 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site3 JP-10/BO** | | **vdW1 Site4 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 25.01 | | ν2 | 28.00 | | ν3 | 41.77 | | ν4 | 46.94 | | ν5 | 64.05 | | ν6 | 135.45 | | ν7 | 179.86 | | ν8 | 261.58 | | ν9 | 318.68 | | ν10 | 332.37 | | ν11 | 404.34 | | ν12 | 496.04 | | ν13 | 533.01 | | ν14 | 556.38 | | ν15 | 668.86 | | ν16 | 752.97 | | ν17 | 766.82 | | ν18 | 811.44 | | ν19 | 843.38 | | ν20 | 881.78 | | ν21 | 883.10 | | ν22 | 916.33 | | ν23 | 918.53 | | ν24 | 941.18 | | ν25 | 942.64 | | ν26 | 952.35 | | ν27 | 985.14 | | ν28 | 985.58 | | ν29 | 1020.62 | | ν30 | 1028.52 | | ν31 | 1066.24 | | ν32 | 1069.03 | | ν33 | 1075.24 | | ν34 | 1076.52 | | ν35 | 1095.19 | | ν36 | 1155.16 | | ν37 | 1170.51 | | ν38 | 1183.65 | | ν39 | 1215.19 | | ν40 | 1221.53 | | ν41 | 1227.43 | | ν42 | 1245.21 | | ν43 | 1270.57 | | ν44 | 1287.39 | | ν45 | 1294.04 | | ν46 | 1307.14 | | ν47 | 1319.85 | | ν48 | 1326.67 | | ν49 | 1334.37 | | ν50 | 1342.10 | | ν51 | 1345.50 | | ν52 | 1363.09 | | ν53 | 1364.93 | | ν54 | 1384.20 | | ν55 | 1387.91 | | ν56 | 1522.93 | | ν57 | 1524.98 | | ν58 | 1529.17 | | ν59 | 1533.93 | | ν60 | 1547.80 | | ν61 | 1561.58 | | ν62 | 1912.43 | | ν63 | 3067.19 | | ν64 | 3070.53 | | ν65 | 3076.30 | | ν66 | 3081.66 | | ν67 | 3083.58 | | ν68 | 3083.90 | | ν69 | 3086.31 | | ν70 | 3087.54 | | ν71 | 3109.52 | | ν72 | 3115.30 | | ν73 | 3126.19 | | ν74 | 3129.34 | | ν75 | 3139.88 | | ν76 | 3145.70 | | ν77 | 3147.60 | | ν78 | 3165.10 | | | |  | | --- | | 10.4022 | | 11.5204 | | 7.9948 | | 6.0032 | | 0.3331 | | 0.0037 | | 0.055 | | 0.0464 | | 0.0704 | | 0.4163 | | 0.0015 | | 0.4425 | | 0.2006 | | 1.5601 | | 0.8299 | | 0.3057 | | 0.7244 | | 0.9059 | | 0.8877 | | 1.0873 | | 2.134 | | 0.0837 | | 0.9403 | | 0.0819 | | 1.5474 | | 1.4747 | | 2.3203 | | 0.3339 | | 2.0433 | | 1.4683 | | 0.0209 | | 0.2565 | | 0.0453 | | 0.0612 | | 0.8208 | | 0.1692 | | 0.2051 | | 1.6119 | | 0.1903 | | 0.0875 | | 2.3233 | | 1.3383 | | 0.022 | | 3.0537 | | 0.7719 | | 0.0025 | | 0.0501 | | 0.3669 | | 0.2287 | | 5.7711 | | 0.0122 | | 0.283 | | 2.1027 | | 3.3765 | | 0.1504 | | 1.3474 | | 2.642 | | 2.8966 | | 8.6984 | | 9.8724 | | 5.5376 | | 143.8152 | | 3.1403 | | 37.0701 | | 23.1113 | | 31.5678 | | 45.566 | | 28.7217 | | 69.2393 | | 3.6115 | | 87.9164 | | 10.3601 | | 0.2336 | | 28.9391 | | 20.677 | | 15.8691 | | 99.8642 | | 11.9742 | | |  | | --- | | 27.76 | | 29.79 | | 33.53 | | 42.94 | | 55.95 | | 128.21 | | 187.85 | | 262.06 | | 318.97 | | 330.55 | | 403.79 | | 492.75 | | 532.80 | | 557.69 | | 669.81 | | 753.19 | | 765.81 | | 810.27 | | 841.09 | | 881.85 | | 882.77 | | 913.96 | | 918.06 | | 941.04 | | 941.19 | | 952.17 | | 980.35 | | 986.15 | | 1021.61 | | 1025.25 | | 1063.95 | | 1068.00 | | 1074.37 | | 1078.78 | | 1095.78 | | 1150.17 | | 1168.50 | | 1183.11 | | 1217.11 | | 1221.45 | | 1226.57 | | 1244.32 | | 1270.01 | | 1282.57 | | 1291.74 | | 1305.02 | | 1317.35 | | 1324.64 | | 1331.12 | | 1341.09 | | 1341.80 | | 1364.87 | | 1373.41 | | 1377.23 | | 1380.13 | | 1523.98 | | 1525.14 | | 1526.82 | | 1536.87 | | 1547.60 | | 1557.81 | | 1914.12 | | 3054.60 | | 3070.51 | | 3072.68 | | 3073.16 | | 3077.45 | | 3087.39 | | 3088.58 | | 3090.13 | | 3113.51 | | 3119.03 | | 3126.51 | | 3132.06 | | 3134.51 | | 3146.25 | | 3151.14 | | 3155.33 | | |  | | --- | | 8.8529 | | 7.5264 | | 0.7163 | | 42.7611 | | 1.9084 | | 0.0162 | | 0.2858 | | 0.1114 | | 0.0705 | | 0.0201 | | 0.0599 | | 0.4325 | | 0.228 | | 1.0373 | | 0.8783 | | 0.3022 | | 0.6634 | | 1.5409 | | 0.9672 | | 1.9589 | | 0.6132 | | 0.2055 | | 0.5606 | | 0.0333 | | 1.0092 | | 1.2621 | | 3.2247 | | 0.3965 | | 2.0061 | | 1.1128 | | 0.0056 | | 0.1429 | | 0.0326 | | 0.1377 | | 0.7191 | | 0.2554 | | 0.0679 | | 1.1836 | | 0.3799 | | 0.0594 | | 3.7636 | | 1.3509 | | 0.0383 | | 0.8493 | | 1.4175 | | 0.0011 | | 0.1921 | | 0.3111 | | 0.9038 | | 5.5236 | | 0.353 | | 1.0352 | | 0.3437 | | 2.9754 | | 0.3432 | | 0.107 | | 4.6663 | | 1.9742 | | 9.136 | | 16.9774 | | 6.0959 | | 72.1057 | | 6.0678 | | 57.631 | | 28.1118 | | 38.3365 | | 24.1082 | | 64.9358 | | 25.933 | | 26.3741 | | 71.4722 | | 7.8932 | | 1.4997 | | 34.4639 | | 25.672 | | 55.5298 | | 28.813 | | 43.8505 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site5 JP-10/BO** | | **vdW1 Site6 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 16.32 | | ν2 | 31.83 | | ν3 | 46.61 | | ν4 | 55.42 | | ν5 | 60.91 | | ν6 | 131.47 | | ν7 | 180.22 | | ν8 | 261.98 | | ν9 | 319.24 | | ν10 | 332.25 | | ν11 | 403.18 | | ν12 | 492.59 | | ν13 | 532.41 | | ν14 | 556.82 | | ν15 | 668.73 | | ν16 | 751.91 | | ν17 | 766.29 | | ν18 | 811.31 | | ν19 | 844.97 | | ν20 | 881.58 | | ν21 | 882.66 | | ν22 | 913.85 | | ν23 | 918.38 | | ν24 | 939.25 | | ν25 | 941.89 | | ν26 | 955.36 | | ν27 | 980.72 | | ν28 | 986.92 | | ν29 | 1019.90 | | ν30 | 1028.42 | | ν31 | 1063.41 | | ν32 | 1069.73 | | ν33 | 1075.96 | | ν34 | 1079.10 | | ν35 | 1094.24 | | ν36 | 1149.74 | | ν37 | 1166.88 | | ν38 | 1185.99 | | ν39 | 1217.66 | | ν40 | 1219.59 | | ν41 | 1227.93 | | ν42 | 1244.58 | | ν43 | 1269.96 | | ν44 | 1285.21 | | ν45 | 1291.27 | | ν46 | 1307.71 | | ν47 | 1320.69 | | ν48 | 1326.41 | | ν49 | 1330.24 | | ν50 | 1340.55 | | ν51 | 1342.21 | | ν52 | 1361.93 | | ν53 | 1363.41 | | ν54 | 1384.43 | | ν55 | 1389.02 | | ν56 | 1523.41 | | ν57 | 1523.82 | | ν58 | 1528.72 | | ν59 | 1533.32 | | ν60 | 1547.08 | | ν61 | 1557.54 | | ν62 | 1913.15 | | ν63 | 3071.47 | | ν64 | 3072.62 | | ν65 | 3073.58 | | ν66 | 3075.95 | | ν67 | 3076.74 | | ν68 | 3085.69 | | ν69 | 3087.27 | | ν70 | 3096.53 | | ν71 | 3101.79 | | ν72 | 3115.71 | | ν73 | 3124.94 | | ν74 | 3130.40 | | ν75 | 3138.37 | | ν76 | 3145.73 | | ν77 | 3147.38 | | ν78 | 3154.53 | | | |  | | --- | | 4.7766 | | 8.8446 | | 2.4556 | | 40.045 | | 4.9459 | | 0.021 | | 0.0019 | | 0.0167 | | 0.0857 | | 0.0609 | | 0.059 | | 0.351 | | 0.2932 | | 0.5982 | | 0.9191 | | 0.4196 | | 0.5512 | | 0.8836 | | 0.8828 | | 2.0695 | | 1.0606 | | 0.142 | | 0.5651 | | 0.0405 | | 1.541 | | 1.6284 | | 3.0369 | | 0.9147 | | 2.1362 | | 1.1878 | | 0.0737 | | 0.2694 | | 0.077 | | 0.0545 | | 0.6561 | | 0.14 | | 0.0555 | | 2.2576 | | 0.05 | | 0.0091 | | 3.2541 | | 2.428 | | 0.0072 | | 1.5747 | | 0.9021 | | 0.0672 | | 0.0825 | | 0.5504 | | 0.9209 | | 4.2151 | | 1.899 | | 0.884 | | 2.2728 | | 1.8569 | | 0.5162 | | 0.1357 | | 2.1706 | | 2.7789 | | 10.4657 | | 13.6939 | | 5.9277 | | 73.6334 | | 17.8843 | | 10.6228 | | 25.164 | | 37.6267 | | 6.2658 | | 39.5679 | | 48.5005 | | 55.3004 | | 62.7507 | | 26.9262 | | 3.1015 | | 31.0599 | | 29.4067 | | 2.197 | | 90.2866 | | 32.6233 | | |  | | --- | | 25.22 | | 28.20 | | 41.87 | | 47.00 | | 64.04 | | 135.43 | | 179.85 | | 261.57 | | 318.68 | | 332.36 | | 404.33 | | 496.04 | | 533.01 | | 556.37 | | 668.85 | | 752.97 | | 766.82 | | 811.44 | | 843.38 | | 881.78 | | 883.10 | | 916.33 | | 918.53 | | 941.18 | | 942.64 | | 952.36 | | 985.13 | | 985.58 | | 1020.61 | | 1028.52 | | 1066.23 | | 1069.03 | | 1075.24 | | 1076.52 | | 1095.19 | | 1155.15 | | 1170.51 | | 1183.65 | | 1215.19 | | 1221.52 | | 1227.43 | | 1245.21 | | 1270.57 | | 1287.39 | | 1294.04 | | 1307.14 | | 1319.85 | | 1326.67 | | 1334.36 | | 1342.10 | | 1345.50 | | 1363.09 | | 1364.93 | | 1384.20 | | 1387.91 | | 1522.93 | | 1524.98 | | 1529.17 | | 1533.93 | | 1547.80 | | 1561.58 | | 1912.40 | | 3067.20 | | 3070.54 | | 3076.31 | | 3081.67 | | 3083.60 | | 3083.91 | | 3086.32 | | 3087.54 | | 3109.53 | | 3115.32 | | 3126.20 | | 3129.36 | | 3139.89 | | 3145.71 | | 3147.62 | | 3165.13 | | |  | | --- | | 10.239 | | 11.3984 | | 8.1581 | | 6.1256 | | 0.3345 | | 0.0037 | | 0.0551 | | 0.0464 | | 0.0704 | | 0.4163 | | 0.0015 | | 0.4427 | | 0.2006 | | 1.5598 | | 0.83 | | 0.3058 | | 0.7243 | | 0.9059 | | 0.8877 | | 1.0872 | | 2.1341 | | 0.0836 | | 0.9404 | | 0.0819 | | 1.5476 | | 1.4742 | | 2.3208 | | 0.3339 | | 2.0433 | | 1.4681 | | 0.0209 | | 0.2565 | | 0.0453 | | 0.0612 | | 0.8205 | | 0.1692 | | 0.2051 | | 1.6121 | | 0.1902 | | 0.0874 | | 2.3233 | | 1.3382 | | 0.022 | | 3.0534 | | 0.7717 | | 0.0024 | | 0.0501 | | 0.3669 | | 0.2283 | | 5.7714 | | 0.0121 | | 0.2831 | | 2.1023 | | 3.3757 | | 0.1506 | | 1.3483 | | 2.6418 | | 2.8966 | | 8.6978 | | 9.8723 | | 5.5387 | | 143.8216 | | 3.1392 | | 37.0656 | | 23.112 | | 31.6052 | | 45.5824 | | 28.745 | | 69.2064 | | 3.5952 | | 87.9156 | | 10.3572 | | 0.2337 | | 28.9492 | | 20.6622 | | 15.9342 | | 99.7907 | | 11.9697 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS1 JP-10/BO** | | **TS2 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -1403.20 | | ν2 | 30.82 | | ν3 | 31.71 | | ν4 | 114.58 | | ν5 | 151.14 | | ν6 | 162.42 | | ν7 | 186.72 | | ν8 | 244.15 | | ν9 | 305.22 | | ν10 | 335.62 | | ν11 | 378.85 | | ν12 | 494.34 | | ν13 | 502.54 | | ν14 | 547.68 | | ν15 | 566.99 | | ν16 | 670.14 | | ν17 | 755.57 | | ν18 | 777.29 | | ν19 | 815.53 | | ν20 | 871.53 | | ν21 | 882.88 | | ν22 | 899.00 | | ν23 | 915.67 | | ν24 | 928.88 | | ν25 | 937.41 | | ν26 | 941.71 | | ν27 | 953.21 | | ν28 | 981.37 | | ν29 | 988.23 | | ν30 | 1017.70 | | ν31 | 1035.44 | | ν32 | 1056.25 | | ν33 | 1064.96 | | ν34 | 1069.48 | | ν35 | 1077.05 | | ν36 | 1110.18 | | ν37 | 1149.58 | | ν38 | 1169.32 | | ν39 | 1184.25 | | ν40 | 1206.50 | | ν41 | 1216.86 | | ν42 | 1222.50 | | ν43 | 1242.35 | | ν44 | 1249.38 | | ν45 | 1282.08 | | ν46 | 1287.79 | | ν47 | 1298.88 | | ν48 | 1309.08 | | ν49 | 1322.19 | | ν50 | 1333.13 | | ν51 | 1337.94 | | ν52 | 1340.80 | | ν53 | 1358.38 | | ν54 | 1362.52 | | ν55 | 1364.60 | | ν56 | 1380.46 | | ν57 | 1387.11 | | ν58 | 1520.97 | | ν59 | 1527.21 | | ν60 | 1528.18 | | ν61 | 1539.01 | | ν62 | 1555.52 | | ν63 | 1908.50 | | ν64 | 3066.21 | | ν65 | 3075.46 | | ν66 | 3076.89 | | ν67 | 3077.67 | | ν68 | 3078.00 | | ν69 | 3090.71 | | ν70 | 3093.38 | | ν71 | 3118.12 | | ν72 | 3122.63 | | ν73 | 3126.67 | | ν74 | 3133.45 | | ν75 | 3138.44 | | ν76 | 3143.04 | | ν77 | 3147.22 | | ν78 | 3159.61 | | | |  | | --- | | 168.5055 | | 4.2171 | | 4.1266 | | 2.0527 | | 1.7476 | | 0.616 | | 0.5447 | | 0.3902 | | 0.2981 | | 0.0522 | | 0.1128 | | 0.6457 | | 5.1846 | | 0.1101 | | 0.5367 | | 1.742 | | 0.9736 | | 0.4746 | | 1.2946 | | 0.4167 | | 0.2821 | | 2.1405 | | 0.7131 | | 1.5409 | | 0.4008 | | 0.959 | | 0.5996 | | 2.8485 | | 5.4582 | | 2.3007 | | 2.3098 | | 2.7429 | | 1.2842 | | 0.271 | | 0.1609 | | 3.2893 | | 0.3025 | | 0.628 | | 0.981 | | 4.0002 | | 0.1832 | | 1.5948 | | 0.4329 | | 2.3393 | | 3.3128 | | 1.9528 | | 1.4666 | | 1.4284 | | 0.5659 | | 0.5739 | | 4.9806 | | 1.5645 | | 1.912 | | 0.5659 | | 2.0331 | | 2.4836 | | 0.8399 | | 4.5357 | | 7.4976 | | 3.2984 | | 7.5204 | | 15.9563 | | 142.6126 | | 24.6438 | | 24.4323 | | 10.1929 | | 18.9904 | | 20.9078 | | 41.3083 | | 8.4537 | | 33.4145 | | 18.409 | | 11.471 | | 34.2565 | | 26.3505 | | 17.7946 | | 52.2843 | | 28.4779 | | |  | | --- | | -1519.46 | | 33.27 | | 41.88 | | 130.83 | | 165.00 | | 184.36 | | 187.12 | | 267.66 | | 273.96 | | 326.27 | | 339.31 | | 403.81 | | 495.37 | | 529.41 | | 556.32 | | 663.96 | | 742.45 | | 767.72 | | 816.95 | | 841.70 | | 877.99 | | 881.39 | | 905.78 | | 925.48 | | 938.06 | | 940.59 | | 969.50 | | 978.73 | | 1005.16 | | 1022.19 | | 1027.35 | | 1063.65 | | 1072.13 | | 1082.18 | | 1092.12 | | 1106.66 | | 1152.67 | | 1166.20 | | 1174.95 | | 1208.27 | | 1215.09 | | 1218.80 | | 1237.72 | | 1254.35 | | 1267.28 | | 1284.79 | | 1290.86 | | 1311.48 | | 1319.42 | | 1326.43 | | 1333.85 | | 1335.98 | | 1351.57 | | 1363.99 | | 1377.46 | | 1387.78 | | 1522.26 | | 1522.72 | | 1527.68 | | 1532.94 | | 1545.50 | | 1556.92 | | 1914.96 | | 3076.56 | | 3078.59 | | 3080.19 | | 3081.42 | | 3085.06 | | 3093.60 | | 3097.66 | | 3100.63 | | 3115.79 | | 3134.80 | | 3139.37 | | 3140.02 | | 3149.06 | | 3158.13 | | 3168.90 | | |  | | --- | | 2.9098 | | 2.9417 | | 3.041 | | 0.8193 | | 2.9825 | | 1.0285 | | 2.9685 | | 0.1221 | | 0.5572 | | 0.2026 | | 0.0794 | | 0.1039 | | 0.6331 | | 0.446 | | 0.6983 | | 1.1427 | | 2.4972 | | 6.2292 | | 5.1316 | | 1.4082 | | 1.8481 | | 2.6286 | | 1.0488 | | 1.12 | | 0.5402 | | 1.6842 | | 6.3433 | | 1.973 | | 8.0328 | | 1.0068 | | 2.1113 | | 0.2253 | | 0.3864 | | 0.2487 | | 4.3581 | | 0.3755 | | 2.8121 | | 3.5013 | | 1.1628 | | 8.3286 | | 0.1445 | | 1.9036 | | 8.0875 | | 3.056 | | 0.7909 | | 1.375 | | 0.8809 | | 7.4323 | | 3.5538 | | 1.9677 | | 3.3962 | | 3.1496 | | 2.221 | | 0.172 | | 0.8924 | | 0.4789 | | 2.4123 | | 0.3228 | | 3.3689 | | 11.4094 | | 12.7036 | | 9.4423 | | 100.7352 | | 19.768 | | 27.845 | | 18.1342 | | 1.6148 | | 19.5862 | | 35.0389 | | 40.9224 | | 8.5607 | | 41.9722 | | 27.2253 | | 6.3554 | | 16.0135 | | 38.7967 | | 42.4141 | | 20.7908 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS3 JP-10/BO** | | **TS4 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -1633.90 | | ν2 | 40.25 | | ν3 | 43.92 | | ν4 | 138.19 | | ν5 | 158.07 | | ν6 | 185.94 | | ν7 | 206.77 | | ν8 | 262.74 | | ν9 | 285.00 | | ν10 | 320.34 | | ν11 | 327.63 | | ν12 | 435.59 | | ν13 | 534.78 | | ν14 | 545.19 | | ν15 | 599.55 | | ν16 | 669.03 | | ν17 | 739.03 | | ν18 | 776.40 | | ν19 | 811.30 | | ν20 | 840.26 | | ν21 | 880.94 | | ν22 | 881.23 | | ν23 | 906.53 | | ν24 | 926.21 | | ν25 | 942.13 | | ν26 | 950.37 | | ν27 | 963.71 | | ν28 | 976.84 | | ν29 | 1019.53 | | ν30 | 1023.46 | | ν31 | 1024.79 | | ν32 | 1065.87 | | ν33 | 1072.43 | | ν34 | 1075.99 | | ν35 | 1083.83 | | ν36 | 1095.57 | | ν37 | 1146.78 | | ν38 | 1166.97 | | ν39 | 1185.34 | | ν40 | 1217.17 | | ν41 | 1220.19 | | ν42 | 1221.04 | | ν43 | 1224.96 | | ν44 | 1261.91 | | ν45 | 1266.90 | | ν46 | 1282.70 | | ν47 | 1293.50 | | ν48 | 1316.10 | | ν49 | 1322.52 | | ν50 | 1327.41 | | ν51 | 1337.01 | | ν52 | 1341.70 | | ν53 | 1358.53 | | ν54 | 1363.15 | | ν55 | 1365.64 | | ν56 | 1384.50 | | ν57 | 1387.08 | | ν58 | 1524.25 | | ν59 | 1528.10 | | ν60 | 1528.12 | | ν61 | 1544.28 | | ν62 | 1545.85 | | ν63 | 1910.67 | | ν64 | 3076.47 | | ν65 | 3077.39 | | ν66 | 3082.78 | | ν67 | 3083.38 | | ν68 | 3084.00 | | ν69 | 3090.72 | | ν70 | 3093.49 | | ν71 | 3118.39 | | ν72 | 3127.16 | | ν73 | 3132.74 | | ν74 | 3134.86 | | ν75 | 3136.18 | | ν76 | 3139.08 | | ν77 | 3149.30 | | ν78 | 3154.66 | | | |  | | --- | | 3.6622 | | 2.9962 | | 3.4046 | | 0.0004 | | 2.1508 | | 3.5711 | | 2.6338 | | 0.1365 | | 1.13 | | 0.0744 | | 0.018 | | 0.7685 | | 0.6381 | | 0.3383 | | 5.4477 | | 0.3644 | | 1.5049 | | 0.6683 | | 1.6339 | | 2.354 | | 0.8076 | | 1.0592 | | 0.3934 | | 0 | | 1.8831 | | 0.109 | | 0.4176 | | 0.4274 | | 0.1025 | | 2.6242 | | 2.6189 | | 4.3579 | | 0.0726 | | 0.4392 | | 0.4878 | | 0.8567 | | 1.8672 | | 1.1748 | | 12.7316 | | 0.0437 | | 0.7401 | | 4.5668 | | 1.5079 | | 0.4713 | | 0.1451 | | 1.6829 | | 0.0324 | | 0.1664 | | 0.0697 | | 2.2152 | | 0.4909 | | 2.833 | | 2.3769 | | 0.9666 | | 0.045 | | 2.838 | | 0.3327 | | 3.6314 | | 5.0402 | | 5.3741 | | 0.1761 | | 11.5092 | | 101.1099 | | 3.993 | | 28.7076 | | 23.6819 | | 13.6448 | | 27.2025 | | 10.4046 | | 75.1234 | | 11.6096 | | 45.176 | | 15.5608 | | 15.612 | | 4.2834 | | 22.1071 | | 46.0715 | | 53.6723 | | |  | | --- | | -1260.83 | | 27.22 | | 32.44 | | 109.89 | | 147.59 | | 167.70 | | 194.12 | | 262.24 | | 291.47 | | 321.49 | | 340.83 | | 401.58 | | 499.06 | | 536.27 | | 556.20 | | 684.14 | | 753.40 | | 767.42 | | 816.16 | | 848.05 | | 878.19 | | 890.29 | | 911.21 | | 916.97 | | 933.69 | | 938.84 | | 950.05 | | 980.88 | | 985.90 | | 1022.87 | | 1044.79 | | 1061.90 | | 1074.48 | | 1081.65 | | 1102.86 | | 1113.30 | | 1151.23 | | 1165.93 | | 1186.98 | | 1205.56 | | 1213.15 | | 1233.55 | | 1242.37 | | 1264.89 | | 1271.58 | | 1279.82 | | 1290.26 | | 1292.21 | | 1322.34 | | 1328.55 | | 1332.04 | | 1339.48 | | 1360.16 | | 1362.33 | | 1367.80 | | 1379.67 | | 1513.14 | | 1523.12 | | 1527.76 | | 1532.84 | | 1543.58 | | 1556.48 | | 1905.36 | | 3058.74 | | 3059.40 | | 3077.52 | | 3080.76 | | 3085.99 | | 3087.42 | | 3095.58 | | 3116.33 | | 3120.94 | | 3129.14 | | 3136.30 | | 3138.13 | | 3147.82 | | 3152.42 | | 3155.07 | | |  | | --- | | 83.202 | | 3.5843 | | 3.3641 | | 0.9275 | | 1.056 | | 0.4069 | | 1.5312 | | 0.1205 | | 1.5511 | | 0.039 | | 0.4303 | | 0.1506 | | 0.2289 | | 0.2371 | | 0.6342 | | 0.8315 | | 0.6877 | | 5.9237 | | 0.3454 | | 0.0678 | | 1.5768 | | 3.2153 | | 0.8917 | | 0.2967 | | 3.0381 | | 0.2882 | | 2.1595 | | 3.3916 | | 1.3306 | | 3.6213 | | 1.0582 | | 0.3201 | | 0.6189 | | 0.9545 | | 1.5222 | | 0.8139 | | 1.821 | | 0.7194 | | 1.6718 | | 9.8409 | | 1.3744 | | 3.8621 | | 0.0291 | | 1.1298 | | 0.9668 | | 0.2142 | | 1.8233 | | 0.3492 | | 0.2395 | | 0.4962 | | 2.8922 | | 5.9452 | | 1.4573 | | 1.0827 | | 1.3406 | | 0.7483 | | 6.4575 | | 2.4008 | | 2.2827 | | 12.4447 | | 15.6225 | | 4.8101 | | 132.7458 | | 16.0321 | | 13.4112 | | 16.419 | | 21.3382 | | 20.7994 | | 29.5822 | | 36.1959 | | 21.084 | | 46.6219 | | 16.0643 | | 1.1119 | | 28.5914 | | 15.3983 | | 35.297 | | 46.3146 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS5 JP-10/BO** | | **TS6 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -1471.12 | | ν2 | 32.49 | | ν3 | 38.74 | | ν4 | 106.50 | | ν5 | 143.67 | | ν6 | 169.14 | | ν7 | 190.54 | | ν8 | 234.19 | | ν9 | 292.03 | | ν10 | 327.89 | | ν11 | 398.72 | | ν12 | 437.19 | | ν13 | 504.33 | | ν14 | 535.60 | | ν15 | 598.72 | | ν16 | 701.45 | | ν17 | 755.66 | | ν18 | 770.07 | | ν19 | 814.91 | | ν20 | 848.60 | | ν21 | 874.80 | | ν22 | 888.07 | | ν23 | 918.98 | | ν24 | 931.30 | | ν25 | 942.00 | | ν26 | 951.90 | | ν27 | 966.27 | | ν28 | 982.17 | | ν29 | 986.92 | | ν30 | 1025.61 | | ν31 | 1028.19 | | ν32 | 1064.53 | | ν33 | 1072.10 | | ν34 | 1075.45 | | ν35 | 1094.87 | | ν36 | 1115.15 | | ν37 | 1150.50 | | ν38 | 1160.80 | | ν39 | 1181.71 | | ν40 | 1202.69 | | ν41 | 1218.55 | | ν42 | 1221.02 | | ν43 | 1242.76 | | ν44 | 1257.00 | | ν45 | 1270.73 | | ν46 | 1292.46 | | ν47 | 1297.81 | | ν48 | 1312.62 | | ν49 | 1322.85 | | ν50 | 1329.80 | | ν51 | 1333.59 | | ν52 | 1338.87 | | ν53 | 1341.93 | | ν54 | 1350.67 | | ν55 | 1362.81 | | ν56 | 1381.13 | | ν57 | 1389.39 | | ν58 | 1522.58 | | ν59 | 1526.57 | | ν60 | 1530.39 | | ν61 | 1541.60 | | ν62 | 1556.43 | | ν63 | 1911.02 | | ν64 | 3061.03 | | ν65 | 3069.99 | | ν66 | 3080.34 | | ν67 | 3082.92 | | ν68 | 3088.54 | | ν69 | 3089.59 | | ν70 | 3092.34 | | ν71 | 3115.20 | | ν72 | 3120.50 | | ν73 | 3127.85 | | ν74 | 3133.10 | | ν75 | 3138.57 | | ν76 | 3147.74 | | ν77 | 3152.17 | | ν78 | 3152.70 | | | |  | | --- | | 100.942 | | 3.8424 | | 3.5258 | | 2.5144 | | 0.7238 | | 2.3885 | | 0.8349 | | 0.1508 | | 0.0402 | | 0.0902 | | 0.1502 | | 0.6801 | | 0.2605 | | 1.0319 | | 3.7465 | | 6.5642 | | 0.2918 | | 0.8768 | | 0.4749 | | 1.1562 | | 2.8571 | | 0.7659 | | 0.3918 | | 1.3306 | | 0.6435 | | 1.3903 | | 2.1792 | | 3.8294 | | 0.2321 | | 1.5665 | | 1.5894 | | 0.1258 | | 0.4753 | | 1.1218 | | 1.3885 | | 0.9585 | | 0.0802 | | 1.1004 | | 3.4361 | | 2.1681 | | 1.822 | | 1.2089 | | 0.7786 | | 1.3414 | | 0.0837 | | 1.3845 | | 0.5649 | | 1.2752 | | 1.4772 | | 1.4602 | | 1.1551 | | 3.2494 | | 2.5423 | | 2.3897 | | 1.8574 | | 1.9849 | | 0.5153 | | 2.0515 | | 2.0657 | | 10.8322 | | 15.2547 | | 4.9296 | | 137.2431 | | 8.6494 | | 18.6669 | | 17.143 | | 19.4697 | | 39.2683 | | 3.793 | | 54.7429 | | 61.7967 | | 5.3483 | | 19.3165 | | 0.3997 | | 21.5642 | | 4.88 | | 57.4395 | | 45.884 | | |  | | --- | | -1384.87 | | 22.84 | | 35.65 | | 115.16 | | 115.92 | | 172.52 | | 181.13 | | 263.79 | | 320.20 | | 325.44 | | 408.37 | | 450.34 | | 497.04 | | 535.52 | | 618.52 | | 676.83 | | 750.05 | | 775.95 | | 810.25 | | 841.65 | | 876.62 | | 899.31 | | 916.90 | | 919.30 | | 940.83 | | 944.72 | | 952.38 | | 979.82 | | 986.45 | | 1026.56 | | 1027.46 | | 1066.16 | | 1069.13 | | 1075.78 | | 1094.14 | | 1095.56 | | 1151.35 | | 1164.57 | | 1183.50 | | 1219.10 | | 1230.32 | | 1232.51 | | 1242.03 | | 1268.93 | | 1270.57 | | 1291.64 | | 1301.20 | | 1310.49 | | 1323.65 | | 1326.57 | | 1333.55 | | 1334.87 | | 1349.62 | | 1352.24 | | 1368.45 | | 1385.13 | | 1386.92 | | 1511.40 | | 1517.44 | | 1526.48 | | 1539.00 | | 1556.82 | | 1909.21 | | 3053.11 | | 3054.64 | | 3078.80 | | 3082.69 | | 3087.80 | | 3091.51 | | 3092.49 | | 3114.71 | | 3120.20 | | 3122.04 | | 3122.85 | | 3132.90 | | 3143.18 | | 3147.31 | | 3152.34 | | |  | | --- | | 105.4313 | | 3.4005 | | 3.7634 | | 3.407 | | 1.0033 | | 0.971 | | 0.8875 | | 0.0088 | | 0.4977 | | 0.153 | | 0.314 | | 2.0056 | | 1.2432 | | 0.2106 | | 3.1422 | | 0.4392 | | 0.2892 | | 0.833 | | 1.7571 | | 2.1557 | | 1.0643 | | 1.8768 | | 1.6066 | | 0.551 | | 0.7043 | | 0.5111 | | 1.5034 | | 2.1033 | | 0.369 | | 2.8935 | | 1.9148 | | 0.1377 | | 2.2543 | | 0.004 | | 1.043 | | 0.0089 | | 0.5364 | | 0.0057 | | 0.4492 | | 0.0134 | | 6.0972 | | 0.0049 | | 7.8002 | | 0.2836 | | 19.7531 | | 2.2444 | | 0.3653 | | 0.0513 | | 0.0722 | | 4.2874 | | 3.2241 | | 0.487 | | 2.9386 | | 1.9151 | | 6.1217 | | 1.1584 | | 0.5232 | | 11.0875 | | 1.1378 | | 1.7271 | | 20.9748 | | 5.4228 | | 128.45 | | 15.8746 | | 10.1655 | | 0.0865 | | 20.8039 | | 27.5572 | | 21.2279 | | 45.9977 | | 65.2964 | | 11.9794 | | 25.8958 | | 14.0512 | | 0.0257 | | 31.1123 | | 23.4208 | | 55.2308 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 1 JP-10/BO** | | **vdW2 Site 2 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 10.90 | | ν2 | 19.15 | | ν3 | 51.99 | | ν4 | 78.71 | | ν5 | 87.76 | | ν6 | 153.12 | | ν7 | 180.43 | | ν8 | 284.39 | | ν9 | 313.29 | | ν10 | 330.22 | | ν11 | 391.09 | | ν12 | 491.75 | | ν13 | 509.53 | | ν14 | 551.78 | | ν15 | 590.31 | | ν16 | 668.39 | | ν17 | 758.09 | | ν18 | 780.41 | | ν19 | 804.02 | | ν20 | 811.65 | | ν21 | 815.44 | | ν22 | 880.13 | | ν23 | 883.81 | | ν24 | 914.68 | | ν25 | 923.43 | | ν26 | 930.49 | | ν27 | 941.19 | | ν28 | 955.75 | | ν29 | 960.19 | | ν30 | 982.75 | | ν31 | 1008.82 | | ν32 | 1023.73 | | ν33 | 1037.42 | | ν34 | 1057.37 | | ν35 | 1064.76 | | ν36 | 1075.71 | | ν37 | 1096.46 | | ν38 | 1142.85 | | ν39 | 1164.64 | | ν40 | 1170.69 | | ν41 | 1202.04 | | ν42 | 1216.16 | | ν43 | 1230.38 | | ν44 | 1254.85 | | ν45 | 1272.34 | | ν46 | 1286.46 | | ν47 | 1293.04 | | ν48 | 1306.59 | | ν49 | 1318.21 | | ν50 | 1332.03 | | ν51 | 1342.00 | | ν52 | 1351.87 | | ν53 | 1358.10 | | ν54 | 1362.85 | | ν55 | 1376.92 | | ν56 | 1385.27 | | ν57 | 1511.27 | | ν58 | 1525.37 | | ν59 | 1528.11 | | ν60 | 1537.25 | | ν61 | 1553.99 | | ν62 | 1811.96 | | ν63 | 2892.37 | | ν64 | 3034.60 | | ν65 | 3074.96 | | ν66 | 3076.53 | | ν67 | 3077.08 | | ν68 | 3078.04 | | ν69 | 3093.02 | | ν70 | 3095.80 | | ν71 | 3097.15 | | ν72 | 3118.55 | | ν73 | 3122.87 | | ν74 | 3131.74 | | ν75 | 3137.07 | | ν76 | 3145.93 | | ν77 | 3160.52 | | ν78 | 3219.66 | | | |  | | --- | | 1.7423 | | 1.9005 | | 0.6205 | | 13.2506 | | 15.0544 | | 0.1635 | | 0.2086 | | 1.0903 | | 2.7867 | | 0.0851 | | 1.8314 | | 2.3945 | | 19.2379 | | 0.3829 | | 13.492 | | 0.8488 | | 0.7355 | | 0.5943 | | 6.6028 | | 7.3764 | | 1.4534 | | 0.2778 | | 2.1453 | | 0.3006 | | 0.7171 | | 1.5998 | | 1.2304 | | 0.3167 | | 0.1889 | | 3.5599 | | 0.6915 | | 1.5915 | | 3.3402 | | 0.1764 | | 0.1442 | | 0.1466 | | 1.1931 | | 0.8794 | | 0.2243 | | 0.5909 | | 1.1471 | | 0.2419 | | 0.6329 | | 1.718 | | 1.6815 | | 1.519 | | 2.207 | | 0.6186 | | 0.4994 | | 1.464 | | 1.5703 | | 2.7494 | | 1.0579 | | 0.6981 | | 1.9478 | | 0.5716 | | 5.6874 | | 3.3013 | | 4.0104 | | 7.5938 | | 12.6563 | | 45.2736 | | 3.1071 | | 35.0407 | | 23.067 | | 33.3633 | | 20.0801 | | 1.0983 | | 6.9715 | | 41.8828 | | 28.8342 | | 56.3976 | | 13.1932 | | 32.0241 | | 27.6638 | | 54.7583 | | 27.7594 | | 21.0165 | | |  | | --- | | 8.04 | | 14.96 | | 50.43 | | 74.23 | | 90.02 | | 136.43 | | 179.27 | | 263.80 | | 317.34 | | 331.39 | | 402.37 | | 494.73 | | 521.59 | | 555.72 | | 661.28 | | 730.91 | | 764.03 | | 801.64 | | 808.67 | | 817.57 | | 838.61 | | 856.15 | | 879.04 | | 899.89 | | 913.97 | | 935.57 | | 940.23 | | 957.42 | | 976.11 | | 995.82 | | 1022.63 | | 1026.67 | | 1062.74 | | 1072.34 | | 1079.50 | | 1107.24 | | 1126.73 | | 1158.92 | | 1181.44 | | 1212.56 | | 1214.37 | | 1226.06 | | 1236.38 | | 1251.97 | | 1275.65 | | 1283.91 | | 1302.20 | | 1317.32 | | 1321.80 | | 1327.30 | | 1333.72 | | 1348.05 | | 1363.91 | | 1376.41 | | 1389.48 | | 1521.05 | | 1523.07 | | 1528.17 | | 1532.81 | | 1545.03 | | 1556.62 | | 1810.69 | | 2889.92 | | 3076.07 | | 3077.65 | | 3080.36 | | 3081.34 | | 3084.74 | | 3095.16 | | 3097.71 | | 3102.53 | | 3113.67 | | 3133.24 | | 3138.54 | | 3139.58 | | 3148.27 | | 3159.39 | | 3171.33 | | |  | | --- | | 0.5259 | | 1.9442 | | 0.2882 | | 14.3083 | | 15.7316 | | 0.1699 | | 0.0492 | | 0.1989 | | 0.4557 | | 0.0694 | | 0.0858 | | 0.7179 | | 0.6503 | | 0.5677 | | 1.4542 | | 0.171 | | 0.3294 | | 0.6994 | | 7.0748 | | 7.4708 | | 0.7136 | | 4.6048 | | 0.5096 | | 0.168 | | 0.4276 | | 0.1019 | | 1.9179 | | 2.0693 | | 1.5435 | | 0.4202 | | 0.79 | | 2.8781 | | 0.1963 | | 0.0481 | | 0.2286 | | 0.3734 | | 0.3864 | | 1.384 | | 0.7918 | | 0.2473 | | 0.7338 | | 5.2179 | | 1.9939 | | 3.5809 | | 0.6021 | | 1.4332 | | 2.7443 | | 1.6662 | | 1.2459 | | 2.1155 | | 2.438 | | 1.2017 | | 0.1464 | | 0.575 | | 0.7402 | | 2.3159 | | 0.4551 | | 4.5486 | | 11.4186 | | 12.0487 | | 9.0366 | | 46.8834 | | 3.5118 | | 21.2937 | | 31.1702 | | 10.7315 | | 15.4824 | | 26.3672 | | 28.2804 | | 48.8118 | | 20.2208 | | 36.6237 | | 25.8959 | | 22.7906 | | 6.2804 | | 43.6475 | | 44.4864 | | 24.1231 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 3 JP-10/BO** | | **vdW2 Site 4 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 12.46 | | ν2 | 18.96 | | ν3 | 44.03 | | ν4 | 76.72 | | ν5 | 82.09 | | ν6 | 110.12 | | ν7 | 184.13 | | ν8 | 243.06 | | ν9 | 316.94 | | ν10 | 317.27 | | ν11 | 369.47 | | ν12 | 456.64 | | ν13 | 531.40 | | ν14 | 545.03 | | ν15 | 666.72 | | ν16 | 743.30 | | ν17 | 745.80 | | ν18 | 786.79 | | ν19 | 796.51 | | ν20 | 804.19 | | ν21 | 809.16 | | ν22 | 848.33 | | ν23 | 875.77 | | ν24 | 886.09 | | ν25 | 905.47 | | ν26 | 930.28 | | ν27 | 943.94 | | ν28 | 946.84 | | ν29 | 973.71 | | ν30 | 975.40 | | ν31 | 1018.64 | | ν32 | 1022.79 | | ν33 | 1039.57 | | ν34 | 1065.35 | | ν35 | 1072.03 | | ν36 | 1076.00 | | ν37 | 1096.29 | | ν38 | 1170.96 | | ν39 | 1182.37 | | ν40 | 1208.70 | | ν41 | 1215.94 | | ν42 | 1222.78 | | ν43 | 1225.19 | | ν44 | 1248.73 | | ν45 | 1263.22 | | ν46 | 1283.07 | | ν47 | 1286.67 | | ν48 | 1310.78 | | ν49 | 1320.00 | | ν50 | 1324.59 | | ν51 | 1343.97 | | ν52 | 1344.37 | | ν53 | 1363.38 | | ν54 | 1363.52 | | ν55 | 1378.88 | | ν56 | 1381.19 | | ν57 | 1519.47 | | ν58 | 1523.37 | | ν59 | 1525.98 | | ν60 | 1540.91 | | ν61 | 1544.77 | | ν62 | 1813.21 | | ν63 | 2902.73 | | ν64 | 3074.48 | | ν65 | 3075.53 | | ν66 | 3076.10 | | ν67 | 3076.41 | | ν68 | 3080.77 | | ν69 | 3089.10 | | ν70 | 3091.99 | | ν71 | 3129.33 | | ν72 | 3131.13 | | ν73 | 3132.67 | | ν74 | 3134.12 | | ν75 | 3136.46 | | ν76 | 3145.64 | | ν77 | 3151.63 | | ν78 | 3200.49 | | | |  | | --- | | 2.3083 | | 1.7465 | | 0.1734 | | 12.7347 | | 14.675 | | 0.4675 | | 0.4444 | | 0.0605 | | 0.0777 | | 0.4832 | | 4.138 | | 6.6157 | | 0.6856 | | 1.1894 | | 0.25 | | 17.5152 | | 1.1748 | | 2.9739 | | 7.197 | | 7.457 | | 0.8666 | | 2.2939 | | 0.9018 | | 1.3137 | | 0.6366 | | 0.0056 | | 2.3332 | | 0.2228 | | 0.4926 | | 2.4049 | | 2.2824 | | 1.4667 | | 0.127 | | 0.0561 | | 0.0343 | | 0.5087 | | 1.0037 | | 0.8238 | | 1.8269 | | 1.2738 | | 0.3039 | | 0.7326 | | 1.4818 | | 1.0625 | | 0.655 | | 2.2761 | | 0.0322 | | 0.0013 | | 0.0246 | | 0.4074 | | 2.2717 | | 0.012 | | 0.4937 | | 0.8201 | | 2.9471 | | 0.383 | | 4.6966 | | 1.3611 | | 7.6344 | | 2.1132 | | 7.7065 | | 40.7126 | | 0.3053 | | 30.0001 | | 25.1619 | | 22.7287 | | 0.9433 | | 30.1418 | | 17.7803 | | 69.4078 | | 34.8252 | | 22.0736 | | 0.8343 | | 24.2827 | | 24.514 | | 53.8831 | | 52.7262 | | 23.8061 | | |  | | --- | | 13.16 | | 18.96 | | 55.11 | | 80.88 | | 86.79 | | 121.77 | | 167.67 | | 238.59 | | 299.65 | | 316.21 | | 390.17 | | 486.20 | | 540.56 | | 557.08 | | 630.57 | | 730.58 | | 752.91 | | 811.24 | | 812.26 | | 817.22 | | 838.03 | | 864.68 | | 895.48 | | 902.01 | | 914.90 | | 919.59 | | 933.89 | | 946.56 | | 981.54 | | 982.75 | | 1020.92 | | 1034.94 | | 1059.19 | | 1069.14 | | 1077.37 | | 1113.83 | | 1143.18 | | 1147.49 | | 1171.11 | | 1177.28 | | 1207.52 | | 1230.18 | | 1244.14 | | 1249.96 | | 1266.92 | | 1276.15 | | 1289.45 | | 1320.63 | | 1323.13 | | 1329.75 | | 1334.56 | | 1356.50 | | 1357.69 | | 1368.25 | | 1384.03 | | 1509.16 | | 1521.98 | | 1525.30 | | 1532.10 | | 1541.60 | | 1554.60 | | 1810.16 | | 2878.38 | | 3025.78 | | 3033.51 | | 3076.21 | | 3080.36 | | 3082.32 | | 3083.39 | | 3093.46 | | 3095.09 | | 3120.62 | | 3132.04 | | 3135.55 | | 3136.65 | | 3145.42 | | 3149.46 | | 3155.75 | | |  | | --- | | 1.212 | | 1.4963 | | 1.2326 | | 12.6277 | | 11.6648 | | 1.2487 | | 0.3609 | | 0.3783 | | 0.5982 | | 0.1449 | | 0.032 | | 0.767 | | 0.236 | | 0.8934 | | 3.5491 | | 0.2398 | | 0.4215 | | 5.4244 | | 3.3856 | | 6.846 | | 1.7176 | | 0.7982 | | 1.9243 | | 0.8024 | | 0.6505 | | 0.4807 | | 0.25 | | 1.3287 | | 1.5038 | | 3.3917 | | 1.5263 | | 1.5789 | | 0.2001 | | 0.0621 | | 0.0947 | | 2.1617 | | 0.4684 | | 0.1157 | | 0.0653 | | 0.6736 | | 2.0357 | | 1.3928 | | 2.283 | | 0.6586 | | 0.13 | | 1.157 | | 1.1039 | | 0.3296 | | 0.2706 | | 2.0512 | | 4.7091 | | 1.4581 | | 0.4577 | | 0.8157 | | 0.7363 | | 6.9806 | | 0.9165 | | 2.1274 | | 9.5236 | | 14.1701 | | 4.4979 | | 51.4216 | | 5.7793 | | 24.5265 | | 26.3864 | | 12.5743 | | 17.4293 | | 34.7996 | | 22.4228 | | 53.7379 | | 37.116 | | 46.7307 | | 24.7458 | | 2.2268 | | 33.6631 | | 8.3852 | | 49.9838 | | 48.1098 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW5 Site 5 JP-10/BO** | | **vdW2 Site 6 JP-10/BO** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 12.06 | | ν2 | 16.32 | | ν3 | 44.92 | | ν4 | 61.45 | | ν5 | 86.38 | | ν6 | 122.36 | | ν7 | 139.81 | | ν8 | 257.10 | | ν9 | 292.19 | | ν10 | 316.52 | | ν11 | 368.74 | | ν12 | 402.28 | | ν13 | 499.67 | | ν14 | 535.15 | | ν15 | 620.57 | | ν16 | 745.07 | | ν17 | 763.32 | | ν18 | 769.57 | | ν19 | 794.28 | | ν20 | 799.48 | | ν21 | 813.70 | | ν22 | 846.48 | | ν23 | 861.27 | | ν24 | 888.43 | | ν25 | 918.59 | | ν26 | 935.75 | | ν27 | 951.98 | | ν28 | 954.61 | | ν29 | 977.31 | | ν30 | 986.30 | | ν31 | 1004.63 | | ν32 | 1029.56 | | ν33 | 1045.30 | | ν34 | 1064.91 | | ν35 | 1072.10 | | ν36 | 1091.15 | | ν37 | 1098.21 | | ν38 | 1136.85 | | ν39 | 1154.38 | | ν40 | 1177.44 | | ν41 | 1204.93 | | ν42 | 1226.89 | | ν43 | 1236.53 | | ν44 | 1252.41 | | ν45 | 1264.27 | | ν46 | 1291.76 | | ν47 | 1297.70 | | ν48 | 1310.96 | | ν49 | 1317.00 | | ν50 | 1330.89 | | ν51 | 1332.83 | | ν52 | 1338.53 | | ν53 | 1345.83 | | ν54 | 1365.11 | | ν55 | 1377.85 | | ν56 | 1388.29 | | ν57 | 1511.12 | | ν58 | 1525.37 | | ν59 | 1527.13 | | ν60 | 1543.39 | | ν61 | 1555.13 | | ν62 | 1814.64 | | ν63 | 2906.44 | | ν64 | 3001.15 | | ν65 | 3009.54 | | ν66 | 3080.47 | | ν67 | 3084.89 | | ν68 | 3086.99 | | ν69 | 3089.52 | | ν70 | 3090.17 | | ν71 | 3108.50 | | ν72 | 3115.43 | | ν73 | 3123.42 | | ν74 | 3130.27 | | ν75 | 3143.40 | | ν76 | 3149.57 | | ν77 | 3152.37 | | ν78 | 3223.87 | | | |  | | --- | | 2.8851 | | 2.9613 | | 5.3304 | | 8.4374 | | 12.052 | | 0.3061 | | 0.7437 | | 0.3972 | | 2.9512 | | 1.8189 | | 32.5124 | | 0.4808 | | 0.541 | | 0.1299 | | 0.7962 | | 0.3963 | | 2.6066 | | 0.2419 | | 7.8351 | | 7.3839 | | 0.7819 | | 0.6128 | | 0.7291 | | 1.7767 | | 0.5754 | | 0.237 | | 0.083 | | 1.538 | | 2.372 | | 0.5351 | | 2.3979 | | 1.7672 | | 0.2019 | | 0.1669 | | 0.0979 | | 0.1097 | | 0.8214 | | 0.0402 | | 0.2962 | | 1.0312 | | 0.3439 | | 4.4629 | | 0.4794 | | 0.5829 | | 0.12 | | 1.6305 | | 0.4752 | | 0.5947 | | 0.5844 | | 0.0795 | | 1.5882 | | 1.6737 | | 5.6809 | | 1.2468 | | 2.3669 | | 0.7429 | | 2.4593 | | 2.566 | | 5.3044 | | 16.0419 | | 4.1319 | | 40.6824 | | 0.8494 | | 42.4352 | | 40.5198 | | 21.2368 | | 10.9704 | | 33.5865 | | 19.6049 | | 52.4023 | | 26.706 | | 64.1346 | | 14.9669 | | 0.9723 | | 26.8063 | | 56.7951 | | 26.2656 | | 19.4333 | | |  | | --- | | 20.48 | | 43.97 | | 65.21 | | 78.25 | | 132.79 | | 142.47 | | 155.27 | | 256.59 | | 290.63 | | 328.18 | | 403.33 | | 469.24 | | 504.94 | | 532.91 | | 696.55 | | 700.22 | | 746.77 | | 770.45 | | 777.48 | | 789.48 | | 810.75 | | 841.19 | | 862.72 | | 914.30 | | 920.66 | | 935.40 | | 951.15 | | 952.65 | | 973.26 | | 987.23 | | 991.72 | | 1038.87 | | 1054.19 | | 1066.69 | | 1075.14 | | 1086.50 | | 1099.97 | | 1150.02 | | 1162.60 | | 1169.10 | | 1206.94 | | 1219.51 | | 1233.07 | | 1255.49 | | 1267.84 | | 1288.13 | | 1297.47 | | 1313.36 | | 1323.70 | | 1328.95 | | 1334.74 | | 1335.45 | | 1364.31 | | 1369.90 | | 1379.71 | | 1390.95 | | 1505.67 | | 1512.39 | | 1525.20 | | 1535.33 | | 1555.00 | | 1803.89 | | 2912.17 | | 3002.83 | | 3004.89 | | 3073.93 | | 3079.64 | | 3083.14 | | 3089.23 | | 3090.96 | | 3101.89 | | 3111.69 | | 3116.32 | | 3122.29 | | 3130.35 | | 3143.48 | | 3150.03 | | 3210.44 | | |  | | --- | | 11.9246 | | 0.6539 | | 5.2745 | | 0.4795 | | 0.5041 | | 7.5732 | | 33.2842 | | 0.0117 | | 0.4948 | | 0.019 | | 0.0396 | | 28.4758 | | 5.8117 | | 0.0527 | | 2.0634 | | 2.0929 | | 0.3362 | | 29.0286 | | 10.3227 | | 0.3215 | | 0.8614 | | 1.3818 | | 0.5729 | | 2.3861 | | 0.3921 | | 1.0768 | | 0.5175 | | 1.3993 | | 1.3255 | | 0.4643 | | 2.3896 | | 2.0464 | | 0.0856 | | 0.4797 | | 0.2623 | | 0.0085 | | 0.0886 | | 0.882 | | 0.0054 | | 1.2031 | | 0.4009 | | 0.1697 | | 2.8481 | | 2.9619 | | 0.1865 | | 1.3028 | | 0.2047 | | 0.1162 | | 0.1616 | | 0.092 | | 2.7386 | | 3.6333 | | 0.8069 | | 5.2374 | | 0.5773 | | 0.6731 | | 11.2548 | | 4.2738 | | 1.58 | | 17.7862 | | 5.0743 | | 22.2762 | | 3.2033 | | 23.1778 | | 22.9136 | | 10.4859 | | 17.2548 | | 21.9568 | | 52.4256 | | 44.4523 | | 9.9801 | | 71.4728 | | 20.9991 | | 11.8443 | | 0.137 | | 26.0725 | | 58.7599 | | 29.9922 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 1 JP-10/BO2** | | **vdW1 Site 2 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 20.34 | | ν2 | 25.81 | | ν3 | 34.54 | | ν4 | 40.03 | | ν5 | 53.31 | | ν6 | 135.16 | | ν7 | 181.90 | | ν8 | 265.84 | | ν9 | 321.48 | | ν10 | 333.14 | | ν11 | 405.53 | | ν12 | 445.13 | | ν13 | 489.49 | | ν14 | 495.33 | | ν15 | 533.64 | | ν16 | 556.15 | | ν17 | 668.11 | | ν18 | 751.80 | | ν19 | 766.05 | | ν20 | 811.05 | | ν21 | 841.34 | | ν22 | 881.71 | | ν23 | 882.12 | | ν24 | 913.00 | | ν25 | 918.21 | | ν26 | 939.30 | | ν27 | 941.80 | | ν28 | 952.12 | | ν29 | 964.61 | | ν30 | 982.50 | | ν31 | 989.63 | | ν32 | 1019.76 | | ν33 | 1026.56 | | ν34 | 1063.17 | | ν35 | 1069.03 | | ν36 | 1075.21 | | ν37 | 1077.00 | | ν38 | 1094.13 | | ν39 | 1155.02 | | ν40 | 1167.26 | | ν41 | 1183.64 | | ν42 | 1215.86 | | ν43 | 1219.79 | | ν44 | 1226.69 | | ν45 | 1244.08 | | ν46 | 1271.67 | | ν47 | 1284.60 | | ν48 | 1293.80 | | ν49 | 1306.39 | | ν50 | 1320.80 | | ν51 | 1327.15 | | ν52 | 1331.16 | | ν53 | 1341.80 | | ν54 | 1343.98 | | ν55 | 1362.27 | | ν56 | 1364.92 | | ν57 | 1383.54 | | ν58 | 1388.02 | | ν59 | 1523.17 | | ν60 | 1524.23 | | ν61 | 1527.47 | | ν62 | 1533.95 | | ν63 | 1546.52 | | ν64 | 1558.22 | | ν65 | 2196.34 | | ν66 | 3070.20 | | ν67 | 3074.08 | | ν68 | 3074.28 | | ν69 | 3074.40 | | ν70 | 3079.80 | | ν71 | 3085.30 | | ν72 | 3090.01 | | ν73 | 3096.98 | | ν74 | 3110.84 | | ν75 | 3119.08 | | ν76 | 3128.97 | | ν77 | 3129.43 | | ν78 | 3134.23 | | ν79 | 3143.56 | | ν80 | 3149.82 | | ν81 | 3158.71 | | | |  | | --- | | 0.9436 | | 0.2536 | | 0.1153 | | 2.1405 | | 0.9517 | | 0.0658 | | 0.0045 | | 0.196 | | 0.1562 | | 0.0447 | | 0.095 | | 63.2813 | | 85.475 | | 0.703 | | 0.4134 | | 0.4819 | | 0.852 | | 0.3454 | | 0.605 | | 1.0631 | | 1.0934 | | 1.089 | | 1.3627 | | 0.0973 | | 0.6032 | | 0.0398 | | 1.2317 | | 1.4909 | | 0.0319 | | 3.5683 | | 0.4577 | | 2.1287 | | 1.6946 | | 0.0578 | | 0.2889 | | 0.1913 | | 0.0884 | | 0.6224 | | 0.3245 | | 0.0251 | | 1.3244 | | 0.2398 | | 0.0453 | | 1.8197 | | 2.6267 | | 0.0503 | | 1.3151 | | 0.9986 | | 0.0051 | | 0.2284 | | 0.6269 | | 1.299 | | 2.3669 | | 2.3484 | | 0.6019 | | 1.7016 | | 1.7043 | | 0.4773 | | 1.8977 | | 2.084 | | 2.9108 | | 9.4502 | | 12.8554 | | 4.9139 | | 562.7852 | | 9.5855 | | 22.4667 | | 17.5108 | | 28.958 | | 30.2366 | | 31.2378 | | 62.667 | | 20.1872 | | 72.7232 | | 11.7421 | | 3.5331 | | 35.132 | | 29.871 | | 44.4937 | | 68.6737 | | 27.4565 | | |  | | --- | | 15.97 | | 30.02 | | 50.28 | | 61.26 | | 64.72 | | 132.15 | | 179.79 | | 261.80 | | 319.39 | | 331.76 | | 402.93 | | 431.83 | | 486.15 | | 492.38 | | 532.22 | | 556.73 | | 668.43 | | 751.66 | | 765.95 | | 810.35 | | 843.69 | | 881.24 | | 882.74 | | 913.67 | | 918.58 | | 939.46 | | 942.62 | | 957.93 | | 964.74 | | 980.72 | | 989.08 | | 1020.17 | | 1029.21 | | 1064.92 | | 1069.60 | | 1076.41 | | 1079.53 | | 1093.64 | | 1149.25 | | 1166.16 | | 1189.78 | | 1218.02 | | 1218.88 | | 1227.92 | | 1244.95 | | 1270.22 | | 1286.13 | | 1292.60 | | 1309.67 | | 1320.78 | | 1326.34 | | 1331.04 | | 1340.59 | | 1343.24 | | 1362.68 | | 1363.65 | | 1383.65 | | 1388.36 | | 1522.96 | | 1523.76 | | 1528.34 | | 1533.26 | | 1546.76 | | 1557.35 | | 2065.91 | | 3070.81 | | 3072.01 | | 3073.47 | | 3076.52 | | 3076.91 | | 3081.87 | | 3089.08 | | 3091.90 | | 3096.57 | | 3116.24 | | 3128.91 | | 3131.28 | | 3137.88 | | 3145.58 | | 3149.02 | | 3155.51 | | |  | | --- | | 0.7548 | | 0.3814 | | 0.0495 | | 3.458 | | 0.4665 | | 0.024 | | 0.0001 | | 0.0083 | | 0.1815 | | 0.0622 | | 0.4082 | | 127.7401 | | 33.1337 | | 0.58 | | 0.2073 | | 0.5651 | | 1.108 | | 0.4325 | | 0.5976 | | 0.9188 | | 0.824 | | 1.7024 | | 1.1809 | | 0.1785 | | 0.4137 | | 0.0592 | | 1.4846 | | 1.5389 | | 0.3038 | | 2.8328 | | 1.0767 | | 2.6677 | | 1.2117 | | 0.0042 | | 0.1714 | | 0.0389 | | 0.0832 | | 0.4283 | | 0.3761 | | 0.0608 | | 2.221 | | 0.0396 | | 0.0333 | | 2.9171 | | 2.9157 | | 0.1194 | | 1.7269 | | 0.9689 | | 0.0534 | | 0.0524 | | 0.4692 | | 0.6854 | | 2.629 | | 3.4067 | | 0.8232 | | 2.3338 | | 1.9874 | | 0.2657 | | 0.6025 | | 2.2274 | | 2.6657 | | 10.9987 | | 14.206 | | 5.4252 | | 182.342 | | 0.7691 | | 32.7965 | | 17.4838 | | 19.1837 | | 20.2004 | | 75.2233 | | 47.1133 | | 42.4844 | | 52.6157 | | 30.579 | | 0.5242 | | 29.9857 | | 26.0005 | | 21.3804 | | 71.1596 | | 31.5835 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 3 JP-10/BO2** | | **vdW1 Site 4 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 20.75 | | ν2 | 32.04 | | ν3 | 47.01 | | ν4 | 59.87 | | ν5 | 65.88 | | ν6 | 134.27 | | ν7 | 179.73 | | ν8 | 262.52 | | ν9 | 318.45 | | ν10 | 332.85 | | ν11 | 403.75 | | ν12 | 427.00 | | ν13 | 484.41 | | ν14 | 496.25 | | ν15 | 533.68 | | ν16 | 557.21 | | ν17 | 668.88 | | ν18 | 751.16 | | ν19 | 766.89 | | ν20 | 812.09 | | ν21 | 843.23 | | ν22 | 881.41 | | ν23 | 883.08 | | ν24 | 914.74 | | ν25 | 919.61 | | ν26 | 939.53 | | ν27 | 942.34 | | ν28 | 949.76 | | ν29 | 964.02 | | ν30 | 984.38 | | ν31 | 988.44 | | ν32 | 1021.19 | | ν33 | 1028.53 | | ν34 | 1067.82 | | ν35 | 1069.93 | | ν36 | 1076.54 | | ν37 | 1078.35 | | ν38 | 1094.60 | | ν39 | 1154.91 | | ν40 | 1169.12 | | ν41 | 1186.24 | | ν42 | 1216.32 | | ν43 | 1219.99 | | ν44 | 1227.41 | | ν45 | 1244.59 | | ν46 | 1268.44 | | ν47 | 1285.76 | | ν48 | 1291.65 | | ν49 | 1307.55 | | ν50 | 1320.45 | | ν51 | 1326.66 | | ν52 | 1332.30 | | ν53 | 1339.66 | | ν54 | 1346.33 | | ν55 | 1362.86 | | ν56 | 1364.65 | | ν57 | 1384.20 | | ν58 | 1387.61 | | ν59 | 1523.81 | | ν60 | 1525.47 | | ν61 | 1529.94 | | ν62 | 1533.96 | | ν63 | 1548.12 | | ν64 | 1559.89 | | ν65 | 2041.91 | | ν66 | 3070.95 | | ν67 | 3072.76 | | ν68 | 3075.01 | | ν69 | 3075.37 | | ν70 | 3079.76 | | ν71 | 3080.88 | | ν72 | 3087.34 | | ν73 | 3088.86 | | ν74 | 3102.45 | | ν75 | 3117.25 | | ν76 | 3130.58 | | ν77 | 3131.35 | | ν78 | 3135.89 | | ν79 | 3144.13 | | ν80 | 3150.11 | | ν81 | 3150.37 | | | |  | | --- | | 0.9219 | | 0.3783 | | 0.4521 | | 2.7667 | | 0.491 | | 0.014 | | 0.0352 | | 0.079 | | 0.1115 | | 0.2036 | | 0.2404 | | 131.9233 | | 34.0021 | | 0.951 | | 0.3977 | | 0.5167 | | 0.9533 | | 0.2907 | | 0.8621 | | 1.3837 | | 0.8264 | | 1.0391 | | 1.6915 | | 0.1387 | | 0.4796 | | 0.2061 | | 1.0807 | | 2.6601 | | 0.5064 | | 2.2775 | | 1.5579 | | 2.4364 | | 1.3895 | | 0.017 | | 0.1903 | | 0.1044 | | 0.0997 | | 0.4939 | | 0.6665 | | 0.044 | | 1.5116 | | 0.2817 | | 0.5929 | | 2.6813 | | 1.86 | | 0.051 | | 1.3419 | | 1.7949 | | 0.0383 | | 0.2725 | | 0.621 | | 1.6759 | | 4.2663 | | 1.3667 | | 0.6915 | | 1.1055 | | 1.0007 | | 0.2709 | | 0.864 | | 2.7656 | | 3.2396 | | 8.6776 | | 14.8715 | | 7.1918 | | 139.756 | | 9.6552 | | 7.671 | | 19.1269 | | 40.3906 | | 24.7243 | | 5.0037 | | 35.3116 | | 68.4693 | | 82.0789 | | 25.6752 | | 0.2555 | | 31.6708 | | 29.0988 | | 20.2967 | | 73.0009 | | 22.3482 | | |  | | --- | | 9.61 | | 31.62 | | 43.81 | | 52.00 | | 62.73 | | 127.55 | | 186.99 | | 263.35 | | 319.87 | | 331.21 | | 404.23 | | 429.06 | | 482.47 | | 492.61 | | 533.05 | | 557.12 | | 669.63 | | 754.07 | | 765.06 | | 809.07 | | 840.44 | | 882.11 | | 882.76 | | 913.39 | | 918.69 | | 940.72 | | 941.99 | | 952.20 | | 963.32 | | 980.11 | | 986.37 | | 1021.86 | | 1023.06 | | 1064.29 | | 1067.23 | | 1075.71 | | 1078.36 | | 1095.17 | | 1149.99 | | 1168.42 | | 1184.56 | | 1216.58 | | 1221.00 | | 1228.01 | | 1244.05 | | 1269.67 | | 1282.17 | | 1292.31 | | 1306.89 | | 1316.42 | | 1323.32 | | 1331.67 | | 1341.28 | | 1341.73 | | 1365.29 | | 1369.37 | | 1373.25 | | 1377.75 | | 1523.90 | | 1525.45 | | 1526.72 | | 1536.47 | | 1547.37 | | 1557.89 | | 2069.23 | | 3034.34 | | 3073.75 | | 3074.34 | | 3079.71 | | 3080.75 | | 3085.66 | | 3089.34 | | 3089.64 | | 3114.40 | | 3119.83 | | 3130.39 | | 3131.80 | | 3136.00 | | 3147.95 | | 3149.89 | | 3154.08 | | |  | | --- | | 1.1432 | | 0.0745 | | 0.01 | | 1.3046 | | 2.1252 | | 0.0073 | | 0.4162 | | 0.1054 | | 0.0639 | | 0.0048 | | 0.2542 | | 124.0241 | | 35.1324 | | 0.4981 | | 0.3263 | | 0.513 | | 0.7824 | | 0.2707 | | 0.837 | | 1.1988 | | 0.887 | | 1.835 | | 0.9389 | | 0.17 | | 0.5518 | | 1.1034 | | 0.0721 | | 1.0666 | | 0.353 | | 3.0123 | | 0.4545 | | 2.1949 | | 1.5685 | | 0.0153 | | 0.1364 | | 0.4149 | | 0.148 | | 0.7105 | | 0.3521 | | 0.0639 | | 1.6216 | | 0.404 | | 0.0733 | | 3.0626 | | 1.2218 | | 0.1423 | | 1.0875 | | 1.4734 | | 0.0887 | | 0.1326 | | 0.3379 | | 0.7194 | | 4.1862 | | 1.7961 | | 0.6058 | | 0.3915 | | 2.0629 | | 1.406 | | 0.244 | | 5.7573 | | 1.0896 | | 9.6943 | | 17.9668 | | 6.4064 | | 193.6789 | | 71.4523 | | 21.8116 | | 11.6274 | | 34.1822 | | 46.5685 | | 27.1662 | | 36.3946 | | 42.7428 | | 71.6393 | | 8.5764 | | 0.6074 | | 32.7056 | | 25.4265 | | 2.8309 | | 87.2264 | | 39.1543 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW1 Site 5 JP-10/BO2** | | **vdW1 Site 6 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 28.53 | | ν2 | 33.30 | | ν3 | 45.43 | | ν4 | 51.26 | | ν5 | 63.05 | | ν6 | 68.07 | | ν7 | 225.10 | | ν8 | 260.17 | | ν9 | 265.39 | | ν10 | 326.59 | | ν11 | 408.17 | | ν12 | 433.03 | | ν13 | 484.65 | | ν14 | 488.11 | | ν15 | 493.96 | | ν16 | 630.31 | | ν17 | 722.74 | | ν18 | 752.76 | | ν19 | 793.66 | | ν20 | 815.55 | | ν21 | 817.40 | | ν22 | 853.01 | | ν23 | 858.05 | | ν24 | 908.37 | | ν25 | 915.43 | | ν26 | 930.87 | | ν27 | 946.03 | | ν28 | 955.10 | | ν29 | 964.39 | | ν30 | 973.15 | | ν31 | 985.22 | | ν32 | 1012.62 | | ν33 | 1016.89 | | ν34 | 1051.25 | | ν35 | 1064.63 | | ν36 | 1093.11 | | ν37 | 1107.69 | | ν38 | 1121.12 | | ν39 | 1134.09 | | ν40 | 1155.57 | | ν41 | 1168.44 | | ν42 | 1216.22 | | ν43 | 1221.25 | | ν44 | 1228.54 | | ν45 | 1242.23 | | ν46 | 1270.20 | | ν47 | 1293.20 | | ν48 | 1303.61 | | ν49 | 1310.27 | | ν50 | 1312.73 | | ν51 | 1327.95 | | ν52 | 1331.89 | | ν53 | 1342.38 | | ν54 | 1350.20 | | ν55 | 1354.93 | | ν56 | 1371.25 | | ν57 | 1382.84 | | ν58 | 1392.39 | | ν59 | 1519.20 | | ν60 | 1524.27 | | ν61 | 1529.14 | | ν62 | 1533.71 | | ν63 | 1552.56 | | ν64 | 1566.65 | | ν65 | 2078.03 | | ν66 | 3033.27 | | ν67 | 3073.51 | | ν68 | 3074.28 | | ν69 | 3078.77 | | ν70 | 3089.88 | | ν71 | 3090.47 | | ν72 | 3098.22 | | ν73 | 3103.54 | | ν74 | 3113.79 | | ν75 | 3119.57 | | ν76 | 3123.08 | | ν77 | 3127.87 | | ν78 | 3129.03 | | ν79 | 3150.51 | | ν80 | 3153.64 | | ν81 | 3183.04 | | | |  | | --- | | 1.0958 | | 0.4644 | | 0.208 | | 0.936 | | 1.407 | | 1.0311 | | 0.052 | | 0.1567 | | 0.1535 | | 0.1457 | | 0.2338 | | 127.2996 | | 1.335 | | 37.1899 | | 0.1551 | | 0.7425 | | 0.0601 | | 0.2587 | | 1.1491 | | 0.3097 | | 0.6498 | | 1.4504 | | 1.5324 | | 2.3451 | | 0.6345 | | 0.2049 | | 0.6611 | | 1.0999 | | 0.1458 | | 3.5959 | | 0.3729 | | 0.8548 | | 1.986 | | 0.4794 | | 0.22 | | 0.8416 | | 0.6968 | | 0.15 | | 0.2608 | | 0.2553 | | 0.7361 | | 1.8523 | | 2.2181 | | 0.7912 | | 0.4178 | | 0.4428 | | 0.6644 | | 0.0728 | | 0.4857 | | 0.708 | | 1.6773 | | 1.2402 | | 0.0233 | | 3.7335 | | 0.4854 | | 5.4997 | | 0.0802 | | 0.1539 | | 7.6039 | | 0.3686 | | 3.4855 | | 6.5998 | | 14.5963 | | 9.1657 | | 198.9796 | | 81.8614 | | 26.7473 | | 27.2619 | | 56.0982 | | 24.2537 | | 44.6014 | | 41.6082 | | 9.0607 | | 67.2654 | | 8.8337 | | 16.2387 | | 18.8486 | | 14.6061 | | 19.488 | | 88.903 | | 21.8969 | | |  | | --- | | 20.83 | | 34.81 | | 42.08 | | 45.05 | | 69.76 | | 135.21 | | 191.92 | | 261.35 | | 319.34 | | 334.50 | | 405.10 | | 443.53 | | 487.66 | | 496.42 | | 532.96 | | 555.32 | | 669.04 | | 752.82 | | 766.75 | | 811.58 | | 843.39 | | 881.96 | | 883.19 | | 915.48 | | 918.53 | | 938.36 | | 940.65 | | 951.90 | | 965.52 | | 983.52 | | 985.88 | | 1016.96 | | 1028.92 | | 1066.13 | | 1068.83 | | 1075.04 | | 1076.19 | | 1096.51 | | 1155.59 | | 1170.15 | | 1184.11 | | 1212.97 | | 1221.92 | | 1227.54 | | 1245.27 | | 1270.73 | | 1287.05 | | 1294.86 | | 1307.83 | | 1319.38 | | 1327.19 | | 1335.14 | | 1342.88 | | 1346.58 | | 1363.35 | | 1365.69 | | 1384.88 | | 1388.87 | | 1524.80 | | 1525.26 | | 1527.61 | | 1536.06 | | 1547.60 | | 1561.56 | | 2164.86 | | 3069.73 | | 3071.10 | | 3077.88 | | 3081.27 | | 3081.62 | | 3084.65 | | 3087.76 | | 3089.50 | | 3110.84 | | 3116.59 | | 3123.01 | | 3127.62 | | 3138.43 | | 3144.31 | | 3147.61 | | 3162.23 | | |  | | --- | | 0.8052 | | 1.555 | | 0.5998 | | 0.1373 | | 1.3065 | | 0.0014 | | 0.1202 | | 0.0627 | | 0.085 | | 0.3934 | | 0.0066 | | 60.0162 | | 78.3564 | | 0.8031 | | 0.1993 | | 0.4621 | | 0.854 | | 0.3453 | | 0.4933 | | 0.8921 | | 0.9864 | | 0.7472 | | 2.3177 | | 0.1763 | | 0.908 | | 0.0062 | | 1.5308 | | 1.2808 | | 0.0175 | | 2.1468 | | 0.5098 | | 2.7075 | | 1.3904 | | 0.0293 | | 0.2018 | | 0.0263 | | 0.0614 | | 0.8308 | | 0.2016 | | 0.0436 | | 1.3152 | | 0.3971 | | 0.0697 | | 2.5199 | | 1.0985 | | 0.0969 | | 2.4318 | | 0.8647 | | 0.0042 | | 0.1818 | | 0.3867 | | 0.256 | | 6.2826 | | 0.0783 | | 0.5669 | | 2.2094 | | 3.1248 | | 0.2703 | | 0.9225 | | 3.2556 | | 1.6554 | | 10.2764 | | 10.4087 | | 6.8159 | | 517.1047 | | 3.2967 | | 37.9625 | | 22.8263 | | 40.5674 | | 11.4192 | | 33.6558 | | 71.5806 | | 10.2259 | | 82.5749 | | 10.8463 | | 31.4826 | | 0.3539 | | 23.0962 | | 32.824 | | 84.4018 | | 13.3377 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS1 JP-10/BO2** | | **TS2 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -353.57 | | ν2 | 13.52 | | ν3 | 37.21 | | ν4 | 57.56 | | ν5 | 101.49 | | ν6 | 141.47 | | ν7 | 177.86 | | ν8 | 265.60 | | ν9 | 323.07 | | ν10 | 335.92 | | ν11 | 395.28 | | ν12 | 487.80 | | ν13 | 494.64 | | ν14 | 499.41 | | ν15 | 535.55 | | ν16 | 556.27 | | ν17 | 668.26 | | ν18 | 751.39 | | ν19 | 760.19 | | ν20 | 804.47 | | ν21 | 826.23 | | ν22 | 881.52 | | ν23 | 882.84 | | ν24 | 913.99 | | ν25 | 922.82 | | ν26 | 934.28 | | ν27 | 941.66 | | ν28 | 952.47 | | ν29 | 977.64 | | ν30 | 984.09 | | ν31 | 988.96 | | ν32 | 1016.90 | | ν33 | 1027.45 | | ν34 | 1051.76 | | ν35 | 1064.48 | | ν36 | 1066.93 | | ν37 | 1077.36 | | ν38 | 1091.87 | | ν39 | 1147.44 | | ν40 | 1169.38 | | ν41 | 1170.44 | | ν42 | 1203.59 | | ν43 | 1215.89 | | ν44 | 1216.91 | | ν45 | 1239.72 | | ν46 | 1252.77 | | ν47 | 1282.70 | | ν48 | 1288.15 | | ν49 | 1299.20 | | ν50 | 1310.22 | | ν51 | 1324.91 | | ν52 | 1330.61 | | ν53 | 1337.94 | | ν54 | 1340.30 | | ν55 | 1361.62 | | ν56 | 1362.94 | | ν57 | 1380.80 | | ν58 | 1384.76 | | ν59 | 1418.79 | | ν60 | 1524.08 | | ν61 | 1527.75 | | ν62 | 1532.05 | | ν63 | 1540.92 | | ν64 | 1555.42 | | ν65 | 1911.37 | | ν66 | 2140.48 | | ν67 | 3074.57 | | ν68 | 3076.56 | | ν69 | 3076.96 | | ν70 | 3077.43 | | ν71 | 3083.61 | | ν72 | 3089.63 | | ν73 | 3095.07 | | ν74 | 3121.74 | | ν75 | 3122.90 | | ν76 | 3129.19 | | ν77 | 3133.10 | | ν78 | 3138.03 | | ν79 | 3140.95 | | ν80 | 3146.87 | | ν81 | 3159.50 | | | |  | | --- | | 714.269 | | 1.0207 | | 0 | | 0.8058 | | 3.0469 | | 0.5212 | | 0.75 | | 10.4215 | | 7.6397 | | 0.2924 | | 7.4443 | | 20.9243 | | 22.6648 | | 28.8995 | | 2.2899 | | 1.8574 | | 2.2303 | | 0.6726 | | 14.2664 | | 24.5623 | | 27.5526 | | 0.8154 | | 2.5587 | | 0.2618 | | 4.666 | | 0.4549 | | 0.4547 | | 3.6548 | | 4.4193 | | 20.6829 | | 11.0702 | | 1.9514 | | 3.3068 | | 23.1099 | | 0.8541 | | 9.2612 | | 0.2073 | | 17.2044 | | 4.9641 | | 0.0376 | | 5.2325 | | 6.6443 | | 28.5209 | | 8.8248 | | 1.2848 | | 8.0154 | | 13.7213 | | 2.1518 | | 13.9827 | | 9.2674 | | 0.5909 | | 11.2958 | | 8.6617 | | 45.318 | | 0.7148 | | 2.4903 | | 18.5303 | | 17.3225 | | 149.2531 | | 0.6195 | | 5.1645 | | 13.1338 | | 4.9099 | | 14.4521 | | 2734.1216 | | 3502.3698 | | 19.5082 | | 11.8509 | | 15.0436 | | 29.0116 | | 10.5153 | | 42.2216 | | 14.0073 | | 20.4028 | | 35.7665 | | 9.5282 | | 31.921 | | 27.3972 | | 19.5693 | | 55.5337 | | 30.0649 | | |  | | --- | | -431.02 | | 20.52 | | 45.02 | | 60.90 | | 114.35 | | 139.18 | | 180.09 | | 264.12 | | 319.95 | | 331.80 | | 402.58 | | 459.76 | | 491.38 | | 498.69 | | 527.87 | | 557.25 | | 665.98 | | 743.54 | | 761.74 | | 805.93 | | 840.64 | | 872.64 | | 880.85 | | 906.47 | | 912.93 | | 921.88 | | 939.69 | | 943.72 | | 967.61 | | 975.70 | | 992.82 | | 1008.33 | | 1022.92 | | 1037.63 | | 1061.72 | | 1071.53 | | 1074.15 | | 1088.11 | | 1125.53 | | 1131.12 | | 1173.02 | | 1208.78 | | 1214.31 | | 1217.71 | | 1235.78 | | 1259.16 | | 1271.10 | | 1284.94 | | 1297.56 | | 1313.22 | | 1321.44 | | 1327.45 | | 1330.84 | | 1336.59 | | 1352.69 | | 1364.25 | | 1380.07 | | 1388.39 | | 1522.50 | | 1524.55 | | 1528.69 | | 1533.01 | | 1546.57 | | 1555.41 | | 1825.19 | | 2036.45 | | 3075.66 | | 3076.34 | | 3079.87 | | 3083.92 | | 3087.74 | | 3097.55 | | 3102.75 | | 3104.33 | | 3119.24 | | 3134.71 | | 3140.78 | | 3141.55 | | 3150.23 | | 3160.18 | | 3171.91 | | |  | | --- | | 1140.5985 | | 1.0231 | | 0.0167 | | 0.4577 | | 2.7941 | | 0.7622 | | 0.2268 | | 0.3117 | | 2.1071 | | 0.0653 | | 0.0366 | | 1.2351 | | 0.9338 | | 34.9528 | | 1.5856 | | 0.6991 | | 1.1949 | | 16.8205 | | 48.2176 | | 78.4909 | | 42.7678 | | 135.4473 | | 12.7064 | | 189.1266 | | 34.4594 | | 384.0394 | | 13.1949 | | 24.6921 | | 24.5471 | | 9.4493 | | 0.7745 | | 58.3312 | | 6.9488 | | 15.1515 | | 14.4307 | | 8.1175 | | 4.0294 | | 0.5302 | | 2.7254 | | 42.4255 | | 11.1223 | | 5.2765 | | 5.9926 | | 0.5286 | | 5.9751 | | 4.945 | | 25.5491 | | 2.2464 | | 14.1615 | | 0.3465 | | 10.3123 | | 0.7616 | | 3.5531 | | 4.3799 | | 12.6513 | | 0.1106 | | 2.1113 | | 2.3199 | | 7.6343 | | 6.6636 | | 1.1822 | | 12.9986 | | 25.6779 | | 44.7476 | | 4518.8553 | | 1070.0888 | | 23.9627 | | 10.0893 | | 32.1671 | | 5.6226 | | 25.2329 | | 33.378 | | 26.8312 | | 9.4098 | | 40.0308 | | 27.8202 | | 3.3096 | | 20.0422 | | 34.15 | | 36.2589 | | 21.8838 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS3 JP-10/BO2** | | **TS4 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -598.46 | | ν2 | 4.01 | | ν3 | 52.96 | | ν4 | 68.94 | | ν5 | 98.45 | | ν6 | 138.10 | | ν7 | 191.05 | | ν8 | 262.25 | | ν9 | 318.14 | | ν10 | 333.97 | | ν11 | 404.89 | | ν12 | 440.47 | | ν13 | 501.87 | | ν14 | 532.02 | | ν15 | 548.69 | | ν16 | 575.59 | | ν17 | 666.40 | | ν18 | 741.35 | | ν19 | 761.59 | | ν20 | 808.09 | | ν21 | 839.88 | | ν22 | 868.79 | | ν23 | 874.08 | | ν24 | 894.98 | | ν25 | 911.52 | | ν26 | 922.47 | | ν27 | 939.62 | | ν28 | 943.93 | | ν29 | 969.72 | | ν30 | 977.80 | | ν31 | 998.52 | | ν32 | 1006.33 | | ν33 | 1028.24 | | ν34 | 1034.68 | | ν35 | 1069.81 | | ν36 | 1073.48 | | ν37 | 1076.76 | | ν38 | 1095.77 | | ν39 | 1098.61 | | ν40 | 1156.66 | | ν41 | 1167.01 | | ν42 | 1190.08 | | ν43 | 1215.72 | | ν44 | 1218.72 | | ν45 | 1226.88 | | ν46 | 1236.48 | | ν47 | 1252.44 | | ν48 | 1268.99 | | ν49 | 1287.02 | | ν50 | 1297.72 | | ν51 | 1315.10 | | ν52 | 1321.78 | | ν53 | 1328.57 | | ν54 | 1341.00 | | ν55 | 1349.92 | | ν56 | 1364.53 | | ν57 | 1365.83 | | ν58 | 1386.79 | | ν59 | 1388.18 | | ν60 | 1524.53 | | ν61 | 1528.44 | | ν62 | 1531.70 | | ν63 | 1546.28 | | ν64 | 1547.85 | | ν65 | 1823.62 | | ν66 | 2018.89 | | ν67 | 3076.18 | | ν68 | 3077.78 | | ν69 | 3086.06 | | ν70 | 3088.72 | | ν71 | 3089.28 | | ν72 | 3092.56 | | ν73 | 3095.39 | | ν74 | 3120.46 | | ν75 | 3128.69 | | ν76 | 3133.17 | | ν77 | 3136.48 | | ν78 | 3138.49 | | ν79 | 3144.82 | | ν80 | 3153.08 | | ν81 | 3157.07 | | | |  | | --- | | 2613.3736 | | 1.2498 | | 0.7753 | | 0.0217 | | 2.3663 | | 0.0243 | | 1.9696 | | 0.2443 | | 0.0022 | | 1.4222 | | 21.3434 | | 9.975 | | 32.6751 | | 0.3529 | | 2.5257 | | 1.3343 | | 1.223 | | 0.9027 | | 237.1344 | | 18.2843 | | 44.9816 | | 516.3801 | | 3.849 | | 292.656 | | 0.7225 | | 244.1108 | | 0.4702 | | 17.1511 | | 106.8948 | | 0.5366 | | 19.2268 | | 3.1212 | | 0.9917 | | 0.7055 | | 38.0198 | | 39.6218 | | 0.0539 | | 1.7459 | | 0.4759 | | 1071.0841 | | 0.1975 | | 140.5386 | | 0.0202 | | 0.2615 | | 17.4865 | | 4.1513 | | 3.9375 | | 1.0826 | | 3.6561 | | 0.1574 | | 0.7452 | | 0.232 | | 0.1488 | | 3.8714 | | 12.3793 | | 0.4329 | | 1.4309 | | 11.971 | | 0.3474 | | 3.061 | | 2.3005 | | 4.1626 | | 7.5393 | | 5.4064 | | 3726.754 | | 269.7729 | | 33.1783 | | 2.8305 | | 19.9062 | | 38.6451 | | 14.6822 | | 14.9971 | | 63.465 | | 5.2163 | | 48.4081 | | 7.6666 | | 19.7368 | | 1.4014 | | 17.7647 | | 37.8228 | | 48.3825 | | |  | | --- | | -1193.49 | | 48.67 | | 90.94 | | 115.25 | | 139.35 | | 164.13 | | 185.94 | | 273.70 | | 300.23 | | 319.31 | | 330.97 | | 399.66 | | 485.01 | | 537.73 | | 544.70 | | 552.79 | | 635.46 | | 659.91 | | 728.81 | | 756.08 | | 806.91 | | 842.27 | | 867.92 | | 895.29 | | 899.99 | | 911.88 | | 919.42 | | 935.15 | | 950.18 | | 976.79 | | 987.83 | | 1022.56 | | 1032.87 | | 1053.47 | | 1061.16 | | 1077.34 | | 1079.71 | | 1101.72 | | 1123.29 | | 1149.31 | | 1152.27 | | 1164.40 | | 1180.30 | | 1208.67 | | 1223.32 | | 1235.49 | | 1245.58 | | 1266.92 | | 1273.24 | | 1286.70 | | 1296.67 | | 1324.29 | | 1327.09 | | 1330.25 | | 1341.93 | | 1361.02 | | 1364.33 | | 1367.29 | | 1373.41 | | 1493.64 | | 1523.01 | | 1533.06 | | 1534.29 | | 1542.65 | | 1559.52 | | 1905.65 | | 3049.70 | | 3064.83 | | 3081.29 | | 3093.70 | | 3096.15 | | 3096.82 | | 3107.40 | | 3133.35 | | 3141.79 | | 3145.98 | | 3152.97 | | 3156.77 | | 3159.07 | | 3163.25 | | 3177.76 | | |  | | --- | | 7068.8658 | | 1.9946 | | 0.8584 | | 0.747 | | 0.7877 | | 0.7787 | | 0.1585 | | 3.638 | | 172.7633 | | 0.2176 | | 0.7069 | | 3.4039 | | 13.8318 | | 0.8758 | | 21.217 | | 7.5925 | | 46.8972 | | 473.203 | | 18.1062 | | 6.6702 | | 4.8924 | | 4.4096 | | 22.8953 | | 19.1843 | | 9.4882 | | 7.8363 | | 1.7442 | | 0.8504 | | 4.9465 | | 6.5681 | | 2.6951 | | 16.6795 | | 34.4613 | | 8.1773 | | 14.9356 | | 4.5156 | | 11.4647 | | 3.2329 | | 50.2939 | | 34.1829 | | 49.2051 | | 18.9625 | | 117.3081 | | 0.9236 | | 80.2033 | | 40.8791 | | 3.2944 | | 4.1175 | | 0.9694 | | 5.2659 | | 3.1309 | | 6.942 | | 0.1646 | | 24.2915 | | 7.7687 | | 6.3394 | | 3.0567 | | 2.3826 | | 1.4958 | | 11.5595 | | 2.1074 | | 10.9166 | | 6.7091 | | 11.9074 | | 6.443 | | 1013.4951 | | 5.2 | | 4.0082 | | 16.3308 | | 30.8617 | | 18.9003 | | 14.478 | | 31.0499 | | 29.2331 | | 7.0105 | | 25.0211 | | 23.9547 | | 6.2124 | | 3.3032 | | 16.746 | | 11.0528 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **TS5 JP-10/BO2** | | **TS6 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | -466.92 | | ν2 | 19.95 | | ν3 | 46.34 | | ν4 | 63.44 | | ν5 | 74.32 | | ν6 | 122.41 | | ν7 | 216.83 | | ν8 | 249.79 | | ν9 | 261.40 | | ν10 | 313.76 | | ν11 | 403.29 | | ν12 | 467.26 | | ν13 | 493.44 | | ν14 | 497.09 | | ν15 | 513.69 | | ν16 | 624.93 | | ν17 | 721.62 | | ν18 | 753.43 | | ν19 | 776.82 | | ν20 | 807.97 | | ν21 | 819.91 | | ν22 | 844.43 | | ν23 | 855.77 | | ν24 | 899.47 | | ν25 | 917.51 | | ν26 | 930.68 | | ν27 | 936.92 | | ν28 | 955.77 | | ν29 | 972.01 | | ν30 | 984.02 | | ν31 | 988.22 | | ν32 | 1010.27 | | ν33 | 1018.26 | | ν34 | 1049.86 | | ν35 | 1065.13 | | ν36 | 1086.77 | | ν37 | 1092.25 | | ν38 | 1113.28 | | ν39 | 1129.17 | | ν40 | 1151.28 | | ν41 | 1167.08 | | ν42 | 1210.45 | | ν43 | 1214.47 | | ν44 | 1222.64 | | ν45 | 1235.15 | | ν46 | 1254.51 | | ν47 | 1268.28 | | ν48 | 1292.10 | | ν49 | 1304.70 | | ν50 | 1307.50 | | ν51 | 1327.15 | | ν52 | 1329.40 | | ν53 | 1332.43 | | ν54 | 1342.46 | | ν55 | 1344.37 | | ν56 | 1370.03 | | ν57 | 1388.54 | | ν58 | 1392.49 | | ν59 | 1431.96 | | ν60 | 1521.26 | | ν61 | 1526.71 | | ν62 | 1530.14 | | ν63 | 1546.71 | | ν64 | 1561.55 | | ν65 | 1915.76 | | ν66 | 2137.98 | | ν67 | 3079.67 | | ν68 | 3082.56 | | ν69 | 3088.61 | | ν70 | 3091.15 | | ν71 | 3091.88 | | ν72 | 3098.07 | | ν73 | 3107.30 | | ν74 | 3112.57 | | ν75 | 3115.72 | | ν76 | 3121.11 | | ν77 | 3130.84 | | ν78 | 3134.53 | | ν79 | 3150.78 | | ν80 | 3153.49 | | ν81 | 3176.90 | | | |  | | --- | | 929.7386 | | 0.6479 | | 0.2416 | | 1.1027 | | 0.3607 | | 1.1518 | | 4.7075 | | 0.1696 | | 4.7222 | | 3.0366 | | 0.9551 | | 12.0459 | | 9.2232 | | 37.1421 | | 44.7684 | | 14.0362 | | 15.6516 | | 0.3004 | | 48.0554 | | 8.2922 | | 4.0948 | | 9.2077 | | 1.4974 | | 26.7708 | | 0.6384 | | 6.9754 | | 10.236 | | 1.3781 | | 3.5037 | | 3.3598 | | 6.8578 | | 3.4649 | | 3.8354 | | 4.482 | | 12.9456 | | 46.0536 | | 3.6014 | | 0.4101 | | 0.0504 | | 3.4359 | | 11.2787 | | 71.951 | | 6.6378 | | 4.2143 | | 10.3687 | | 6.5392 | | 9.0582 | | 3.7722 | | 3.6122 | | 4.0491 | | 5.1019 | | 1.893 | | 3.2515 | | 0.433 | | 40.3078 | | 2.8216 | | 1.3038 | | 0.4309 | | 9.1013 | | 3.6064 | | 2.3065 | | 18.4365 | | 25.325 | | 6.8702 | | 1683.2422 | | 2740.6255 | | 22.4465 | | 13.7615 | | 14.0221 | | 12.3689 | | 50.7095 | | 22.485 | | 10.7894 | | 5.9518 | | 91.5297 | | 9.4178 | | 13.6385 | | 0.1945 | | 18.928 | | 65.1627 | | 19.9361 | | |  | | --- | | -2114.01 | | 49.41 | | 67.38 | | 103.87 | | 126.60 | | 187.41 | | 224.29 | | 254.75 | | 295.66 | | 326.42 | | 346.57 | | 409.52 | | 491.85 | | 504.68 | | 535.81 | | 595.37 | | 704.92 | | 718.20 | | 737.11 | | 774.38 | | 813.94 | | 824.50 | | 846.51 | | 863.85 | | 907.94 | | 919.39 | | 923.40 | | 949.93 | | 955.90 | | 969.27 | | 988.25 | | 1004.89 | | 1014.58 | | 1041.68 | | 1064.74 | | 1067.76 | | 1077.21 | | 1093.46 | | 1110.57 | | 1142.35 | | 1160.31 | | 1172.27 | | 1214.85 | | 1226.67 | | 1237.70 | | 1242.96 | | 1263.57 | | 1272.92 | | 1288.36 | | 1298.52 | | 1310.19 | | 1318.80 | | 1326.92 | | 1328.90 | | 1338.98 | | 1344.10 | | 1354.01 | | 1373.36 | | 1384.39 | | 1394.83 | | 1486.53 | | 1497.01 | | 1527.36 | | 1541.14 | | 1562.60 | | 1919.70 | | 3037.01 | | 3055.15 | | 3083.31 | | 3090.15 | | 3092.71 | | 3101.47 | | 3103.45 | | 3110.69 | | 3117.06 | | 3118.53 | | 3133.85 | | 3140.59 | | 3150.09 | | 3152.94 | | 3187.62 | | |  | | --- | | 15943.5411 | | 2.393 | | 0.7971 | | 1.9112 | | 0.6714 | | 3.6182 | | 5.8467 | | 2.3392 | | 5.8954 | | 0.2172 | | 66.6118 | | 0.8072 | | 0.5514 | | 0.4628 | | 40.2445 | | 181.2974 | | 8.2044 | | 5.2556 | | 5.4287 | | 0.2441 | | 0.2624 | | 2.9318 | | 7.974 | | 4.9861 | | 1.1967 | | 2.0103 | | 41.4041 | | 0.5785 | | 0.4046 | | 4.2155 | | 0.712 | | 16.9006 | | 6.7097 | | 28.0866 | | 14.1209 | | 2.2345 | | 15.2452 | | 0.5111 | | 0.5047 | | 2.6469 | | 5.5145 | | 1.7413 | | 72.7411 | | 1.4417 | | 27.8998 | | 21.7862 | | 75.269 | | 10.7697 | | 13.7352 | | 6.0486 | | 4.3417 | | 6.2081 | | 0.3671 | | 12.801 | | 4.0004 | | 1.8739 | | 7.6422 | | 6.7937 | | 1.7097 | | 0.2975 | | 31.3514 | | 6.8118 | | 2.483 | | 12.1193 | | 2.9288 | | 569.444 | | 10.1661 | | 14.1249 | | 19.8876 | | 8.6556 | | 46.1508 | | 18.6811 | | 25.9844 | | 6.4079 | | 34.1603 | | 9.7158 | | 1.5096 | | 5.2697 | | 16.3727 | | 41.8261 | | 14.0649 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW2 Site 1 JP-10/BO2** | | **vdW2 Site 2 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 20.50 | | ν2 | 26.79 | | ν3 | 62.53 | | ν4 | 64.30 | | ν5 | 128.71 | | ν6 | 160.09 | | ν7 | 188.05 | | ν8 | 293.91 | | ν9 | 326.48 | | ν10 | 332.29 | | ν11 | 399.24 | | ν12 | 489.66 | | ν13 | 492.79 | | ν14 | 510.17 | | ν15 | 521.43 | | ν16 | 552.90 | | ν17 | 568.22 | | ν18 | 668.56 | | ν19 | 686.36 | | ν20 | 758.95 | | ν21 | 782.39 | | ν22 | 816.86 | | ν23 | 880.12 | | ν24 | 882.01 | | ν25 | 914.76 | | ν26 | 922.32 | | ν27 | 930.86 | | ν28 | 940.96 | | ν29 | 955.25 | | ν30 | 961.71 | | ν31 | 982.71 | | ν32 | 1010.26 | | ν33 | 1023.27 | | ν34 | 1026.41 | | ν35 | 1035.60 | | ν36 | 1053.98 | | ν37 | 1065.03 | | ν38 | 1073.72 | | ν39 | 1079.25 | | ν40 | 1102.99 | | ν41 | 1150.04 | | ν42 | 1167.80 | | ν43 | 1174.16 | | ν44 | 1203.29 | | ν45 | 1217.16 | | ν46 | 1231.05 | | ν47 | 1254.60 | | ν48 | 1276.54 | | ν49 | 1289.57 | | ν50 | 1295.90 | | ν51 | 1306.83 | | ν52 | 1319.05 | | ν53 | 1333.27 | | ν54 | 1343.28 | | ν55 | 1348.99 | | ν56 | 1359.27 | | ν57 | 1363.48 | | ν58 | 1377.43 | | ν59 | 1386.00 | | ν60 | 1509.03 | | ν61 | 1526.34 | | ν62 | 1528.38 | | ν63 | 1539.14 | | ν64 | 1557.19 | | ν65 | 2062.07 | | ν66 | 3038.20 | | ν67 | 3076.77 | | ν68 | 3078.35 | | ν69 | 3079.32 | | ν70 | 3081.21 | | ν71 | 3095.36 | | ν72 | 3103.91 | | ν73 | 3104.99 | | ν74 | 3123.06 | | ν75 | 3127.57 | | ν76 | 3134.54 | | ν77 | 3140.37 | | ν78 | 3149.16 | | ν79 | 3168.35 | | ν80 | 3198.84 | | ν81 | 3522.17 | | | |  | | --- | | 2.3706 | | 1.4865 | | 0.2913 | | 1.848 | | 4.3932 | | 2.8505 | | 2.2894 | | 2.442 | | 3.6955 | | 0.8125 | | 0.3028 | | 27.9685 | | 17.8878 | | 81.2635 | | 3.2436 | | 7.4453 | | 41.6398 | | 1.2331 | | 72.7748 | | 3.5682 | | 1.8365 | | 1.7802 | | 0.2213 | | 4.6889 | | 0.6505 | | 0.9635 | | 1.3691 | | 0.9506 | | 0.204 | | 0.2359 | | 4.6985 | | 0.4433 | | 22.8335 | | 1.8728 | | 0.7364 | | 7.1745 | | 1.1539 | | 46.435 | | 32.7842 | | 8.6332 | | 3.0302 | | 0.3431 | | 0.8513 | | 0.9288 | | 0.2388 | | 0.5322 | | 2.3723 | | 2.3164 | | 1.1751 | | 2.8415 | | 0.9057 | | 0.5421 | | 1.5956 | | 1.3732 | | 3.9895 | | 0.8176 | | 0.6481 | | 2.302 | | 0.8747 | | 7.8306 | | 4.0125 | | 4.3549 | | 6.8561 | | 14.2639 | | 333.1714 | | 22.1868 | | 22.2034 | | 31.7121 | | 8.7818 | | 12.287 | | 25.6074 | | 1.9017 | | 32.0258 | | 29.5525 | | 14.5785 | | 29.6036 | | 25.0509 | | 48.6414 | | 19.783 | | 18.0309 | | 939.8796 | | |  | | --- | | 7.74 | | 21.55 | | 53.37 | | 63.36 | | 133.04 | | 139.54 | | 178.87 | | 263.65 | | 317.11 | | 331.72 | | 401.57 | | 478.59 | | 486.27 | | 499.09 | | 516.56 | | 521.08 | | 557.16 | | 660.84 | | 725.87 | | 765.21 | | 800.88 | | 839.57 | | 859.24 | | 879.23 | | 900.44 | | 914.27 | | 936.33 | | 942.21 | | 961.23 | | 976.14 | | 997.50 | | 1022.91 | | 1024.86 | | 1028.12 | | 1063.30 | | 1072.48 | | 1077.92 | | 1082.68 | | 1108.96 | | 1126.93 | | 1159.16 | | 1183.56 | | 1214.21 | | 1216.39 | | 1226.96 | | 1237.46 | | 1252.87 | | 1276.41 | | 1285.81 | | 1303.58 | | 1317.26 | | 1322.18 | | 1328.52 | | 1335.78 | | 1350.10 | | 1365.56 | | 1376.46 | | 1390.03 | | 1520.56 | | 1523.12 | | 1530.70 | | 1532.85 | | 1545.65 | | 1557.28 | | 2058.76 | | 3076.74 | | 3080.17 | | 3082.27 | | 3086.06 | | 3089.17 | | 3099.05 | | 3104.84 | | 3107.52 | | 3117.94 | | 3135.80 | | 3144.92 | | 3145.65 | | 3155.61 | | 3165.14 | | 3179.00 | | 3487.35 | | |  | | --- | | 1.0856 | | 1.2096 | | 0.9811 | | 4.1443 | | 6.1822 | | 5.0262 | | 0.1801 | | 0.3976 | | 0.5325 | | 0.057 | | 0.0604 | | 76.4358 | | 29.2379 | | 27.3207 | | 17.3574 | | 3.9195 | | 0.6097 | | 1.6425 | | 0.2849 | | 0.3382 | | 1.0136 | | 1.3396 | | 3.5759 | | 0.7243 | | 0.4342 | | 0.844 | | 0.2399 | | 2.325 | | 2.0639 | | 1.5785 | | 0.4824 | | 1.1234 | | 17.4262 | | 2.5941 | | 0.0504 | | 0.7405 | | 89.1786 | | 43.1928 | | 0.4846 | | 0.9603 | | 2.782 | | 1.4677 | | 1.5716 | | 0.2982 | | 6.0983 | | 2.1883 | | 3.3616 | | 0.4685 | | 2.2081 | | 3.4981 | | 2.1279 | | 0.7077 | | 2.0981 | | 2.845 | | 1.8164 | | 0.4439 | | 0.614 | | 1.0674 | | 2.7043 | | 0.5812 | | 6.2592 | | 11.1794 | | 10.5044 | | 9.2041 | | 298.2644 | | 19.9313 | | 15.7278 | | 27.1933 | | 2.1487 | | 23.6542 | | 30.7729 | | 25.9469 | | 14.7123 | | 36.7172 | | 25.4349 | | 20.277 | | 8.1374 | | 22.7291 | | 32.2116 | | 18.6567 | | 928.0309 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | |  |  |  |
|  | **vdW2 Site 3 JP-10/BO2** | | **vdW1 Site 4 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 12.1168 | | ν2 | 49.6797 | | ν3 | 59.289 | | ν4 | 74.7655 | | ν5 | 115.244 | | ν6 | 125.2828 | | ν7 | 193.7937 | | ν8 | 245.3831 | | ν9 | 316.1639 | | ν10 | 318.4052 | | ν11 | 394.2835 | | ν12 | 452.3282 | | ν13 | 475.5891 | | ν14 | 509.461 | | ν15 | 515.8287 | | ν16 | 532.8848 | | ν17 | 549.0566 | | ν18 | 666.957 | | ν19 | 738.6039 | | ν20 | 774.1267 | | ν21 | 807.1504 | | ν22 | 818.7799 | | ν23 | 863.1253 | | ν24 | 872.8306 | | ν25 | 884.5734 | | ν26 | 903.9749 | | ν27 | 927.178 | | ν28 | 943.5852 | | ν29 | 949.1392 | | ν30 | 968.4874 | | ν31 | 975.6283 | | ν32 | 1020.213 | | ν33 | 1022.797 | | ν34 | 1023.24 | | ν35 | 1041.697 | | ν36 | 1057.218 | | ν37 | 1067.001 | | ν38 | 1072.108 | | ν39 | 1080.11 | | ν40 | 1096.973 | | ν41 | 1167.701 | | ν42 | 1183.156 | | ν43 | 1208.8 | | ν44 | 1219.588 | | ν45 | 1222.979 | | ν46 | 1225.47 | | ν47 | 1247.918 | | ν48 | 1262.791 | | ν49 | 1278.604 | | ν50 | 1287.105 | | ν51 | 1312.581 | | ν52 | 1323.327 | | ν53 | 1325.89 | | ν54 | 1340.032 | | ν55 | 1345.056 | | ν56 | 1363.668 | | ν57 | 1364.432 | | ν58 | 1377.423 | | ν59 | 1380.473 | | ν60 | 1523.474 | | ν61 | 1526.141 | | ν62 | 1528.758 | | ν63 | 1543.467 | | ν64 | 1545.071 | | ν65 | 2063.051 | | ν66 | 3076.225 | | ν67 | 3080.695 | | ν68 | 3081.82 | | ν69 | 3084.158 | | ν70 | 3085.221 | | ν71 | 3093.467 | | ν72 | 3096.666 | | ν73 | 3134.469 | | ν74 | 3136.564 | | ν75 | 3137.628 | | ν76 | 3139.047 | | ν77 | 3139.851 | | ν78 | 3156.055 | | ν79 | 3156.724 | | ν80 | 3173.306 | | ν81 | 3605.203 | | | |  | | --- | | 0.4315 | | 0.8641 | | 3.3385 | | 0.0328 | | 6.587 | | 0.9894 | | 0.4441 | | 0.0104 | | 0.4274 | | 0.1103 | | 2.2733 | | 90.2324 | | 53.4671 | | 20.6341 | | 10.5285 | | 2.6377 | | 1.4981 | | 0.018 | | 1.5339 | | 3.7796 | | 0.2074 | | 11.9918 | | 10.1696 | | 0.6075 | | 4.8868 | | 0.1917 | | 0.0358 | | 1.8465 | | 0.3332 | | 1.1937 | | 3.9225 | | 0.7266 | | 43.8685 | | 4.7183 | | 3.4352 | | 96.7339 | | 0.0597 | | 0.3235 | | 0.6462 | | 2.8208 | | 0.9671 | | 2.1185 | | 0.5052 | | 0.272 | | 0.8852 | | 1.5527 | | 1.7171 | | 0.3915 | | 2.777 | | 0.0081 | | 0.0028 | | 0.1132 | | 0.7342 | | 0.0947 | | 2.8246 | | 1.2661 | | 0.2928 | | 2.2829 | | 0.257 | | 3.4713 | | 4.0334 | | 13.771 | | 0.3833 | | 7.3029 | | 298.9734 | | 20.5125 | | 16.185 | | 3.4178 | | 30.9515 | | 26.6547 | | 25.3843 | | 52.8194 | | 29.2062 | | 1.628 | | 34.2155 | | 12.1862 | | 29.0367 | | 27.1853 | | 37.5725 | | 20.87 | | 840.4576 | | |  | | --- | | 30.41 | | 50.56 | | 57.17 | | 71.76 | | 123.52 | | 138.89 | | 183.79 | | 254.86 | | 306.34 | | 319.89 | | 394.26 | | 487.21 | | 488.91 | | 517.11 | | 536.71 | | 554.82 | | 568.75 | | 645.24 | | 731.20 | | 755.27 | | 810.93 | | 840.70 | | 866.17 | | 897.06 | | 901.86 | | 914.08 | | 920.15 | | 934.00 | | 947.42 | | 979.67 | | 985.07 | | 1022.38 | | 1024.36 | | 1036.56 | | 1059.58 | | 1071.99 | | 1077.99 | | 1090.98 | | 1111.27 | | 1146.54 | | 1150.35 | | 1174.46 | | 1182.47 | | 1206.35 | | 1230.86 | | 1247.09 | | 1253.90 | | 1269.55 | | 1278.52 | | 1291.87 | | 1321.94 | | 1324.12 | | 1330.97 | | 1339.16 | | 1358.49 | | 1359.77 | | 1369.01 | | 1378.52 | | 1505.73 | | 1522.26 | | 1532.79 | | 1533.50 | | 1542.63 | | 1560.09 | | 2055.32 | | 3031.28 | | 3051.85 | | 3079.16 | | 3084.77 | | 3086.51 | | 3089.71 | | 3099.12 | | 3101.38 | | 3126.07 | | 3134.91 | | 3142.66 | | 3143.32 | | 3149.33 | | 3154.18 | | 3161.13 | | 3412.31 | | |  | | --- | | 1.5073 | | 1.8945 | | 2.5573 | | 1.765 | | 1.0062 | | 5.76 | | 3.0695 | | 0.6036 | | 1.5376 | | 0.1568 | | 0.0361 | | 35.5508 | | 0.5968 | | 48.165 | | 4.4233 | | 1.4027 | | 67.2147 | | 5.3149 | | 0.269 | | 0.8696 | | 2.494 | | 2.9125 | | 0.2896 | | 2.4924 | | 1.0059 | | 0.8858 | | 0.5292 | | 0.2371 | | 1.7036 | | 3.9548 | | 2.2087 | | 0.7131 | | 18.0678 | | 5.9431 | | 1.0741 | | 0.8556 | | 5.1316 | | 86.7918 | | 4.8182 | | 3.4955 | | 1.3787 | | 0.5519 | | 0.5706 | | 3.9115 | | 1.2784 | | 1.634 | | 0.3748 | | 0.0308 | | 1.7188 | | 1.7618 | | 0.3022 | | 0.2453 | | 3.2922 | | 4.3833 | | 1.342 | | 0.2758 | | 0.9709 | | 1.6303 | | 8.6751 | | 1.3351 | | 9.5566 | | 4.8621 | | 14.3953 | | 5.3042 | | 286.2429 | | 18.697 | | 6.3082 | | 11.0008 | | 15.927 | | 34.6799 | | 15.7452 | | 39.4447 | | 21.065 | | 39.1885 | | 21.1375 | | 29.1259 | | 3.5653 | | 7.008 | | 36.9329 | | 33.0417 | | 856.9246 | |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | |  |  |  |
|  | **vdW2 Site 5 JP-10/BO2** | | **vdW2 Site 6 JP-10/BO2** | |
| Normal modes | Frequencies(cm-1) | IR Inten | Frequencies(cm-1) | IR Inten |
| |  |  | | --- | --- | | ν1 | 27.40 | | ν2 | 45.09 | | ν3 | 51.58 | | ν4 | 68.84 | | ν5 | 104.21 | | ν6 | 141.22 | | ν7 | 175.29 | | ν8 | 248.17 | | ν9 | 280.97 | | ν10 | 334.43 | | ν11 | 401.33 | | ν12 | 481.18 | | ν13 | 492.57 | | ν14 | 511.08 | | ν15 | 515.39 | | ν16 | 535.40 | | ν17 | 587.15 | | ν18 | 707.74 | | ν19 | 740.38 | | ν20 | 756.58 | | ν21 | 791.40 | | ν22 | 816.46 | | ν23 | 827.09 | | ν24 | 853.10 | | ν25 | 887.54 | | ν26 | 919.45 | | ν27 | 931.50 | | ν28 | 939.22 | | ν29 | 955.82 | | ν30 | 970.15 | | ν31 | 986.01 | | ν32 | 1003.77 | | ν33 | 1020.24 | | ν34 | 1024.51 | | ν35 | 1044.35 | | ν36 | 1064.89 | | ν37 | 1070.34 | | ν38 | 1072.74 | | ν39 | 1093.20 | | ν40 | 1111.23 | | ν41 | 1139.29 | | ν42 | 1160.23 | | ν43 | 1170.52 | | ν44 | 1201.97 | | ν45 | 1226.17 | | ν46 | 1238.61 | | ν47 | 1258.91 | | ν48 | 1271.52 | | ν49 | 1292.68 | | ν50 | 1306.45 | | ν51 | 1312.32 | | ν52 | 1321.21 | | ν53 | 1327.63 | | ν54 | 1333.27 | | ν55 | 1341.83 | | ν56 | 1349.67 | | ν57 | 1368.32 | | ν58 | 1378.60 | | ν59 | 1395.34 | | ν60 | 1512.88 | | ν61 | 1525.86 | | ν62 | 1534.19 | | ν63 | 1544.59 | | ν64 | 1555.69 | | ν65 | 2058.66 | | ν66 | 3031.52 | | ν67 | 3050.84 | | ν68 | 3082.62 | | ν69 | 3083.13 | | ν70 | 3089.98 | | ν71 | 3092.47 | | ν72 | 3094.24 | | ν73 | 3109.09 | | ν74 | 3119.67 | | ν75 | 3124.75 | | ν76 | 3133.92 | | ν77 | 3149.71 | | ν78 | 3152.82 | | ν79 | 3155.65 | | ν80 | 3192.13 | | ν81 | 3541.12 | | | |  | | --- | | 1.0546 | | 0.8708 | | 0.3489 | | 6.7314 | | 0.4027 | | 5.7408 | | 5.2943 | | 0.1633 | | 0.9841 | | 0.664 | | 1.3043 | | 38.6487 | | 6.6547 | | 44.4692 | | 40.1264 | | 38.3458 | | 24.1459 | | 2.0404 | | 0.3705 | | 0.5993 | | 2.1718 | | 0.9598 | | 0.7141 | | 2.9196 | | 2.5107 | | 0.4369 | | 0.5963 | | 0.5357 | | 1.6401 | | 1.3644 | | 0.1588 | | 2.4258 | | 2.1783 | | 22.0734 | | 2.0014 | | 33.3195 | | 5.2737 | | 112.2041 | | 3.1353 | | 0.3612 | | 0.3054 | | 1.3404 | | 0.6394 | | 0.4935 | | 5.3337 | | 1.2298 | | 0.2411 | | 0.4298 | | 1.5302 | | 2.3412 | | 0.0613 | | 1.2255 | | 1.4725 | | 3.5467 | | 0.198 | | 4.734 | | 1.5112 | | 4.2658 | | 0.8608 | | 5.3279 | | 2.5165 | | 12.6938 | | 19.7558 | | 4.245 | | 255.2814 | | 18.0839 | | 14.8272 | | 13.2513 | | 21.2073 | | 26.7757 | | 38.6218 | | 25.6923 | | 7.6225 | | 66.9521 | | 7.7386 | | 0.4968 | | 9.632 | | 46.7784 | | 29.5014 | | 15.9397 | | 712.0001 | | |  | | --- | | 28.35 | | 44.57 | | 53.95 | | 83.08 | | 93.65 | | 125.31 | | 198.11 | | 250.89 | | 269.57 | | 328.17 | | 403.75 | | 472.27 | | 480.19 | | 504.25 | | 509.13 | | 520.77 | | 610.44 | | 723.29 | | 743.27 | | 773.29 | | 779.92 | | 814.68 | | 827.11 | | 850.26 | | 910.39 | | 916.91 | | 931.60 | | 949.38 | | 952.20 | | 957.11 | | 987.77 | | 994.51 | | 1021.22 | | 1024.19 | | 1056.33 | | 1061.03 | | 1064.37 | | 1070.35 | | 1092.70 | | 1109.47 | | 1137.56 | | 1159.94 | | 1169.90 | | 1207.56 | | 1223.43 | | 1234.44 | | 1259.01 | | 1269.42 | | 1283.06 | | 1294.68 | | 1312.92 | | 1317.21 | | 1324.82 | | 1336.00 | | 1343.52 | | 1359.04 | | 1371.34 | | 1383.80 | | 1395.15 | | 1500.17 | | 1507.88 | | 1526.49 | | 1531.17 | | 1554.94 | | 2059.75 | | 3013.63 | | 3031.21 | | 3075.95 | | 3082.11 | | 3088.17 | | 3091.43 | | 3092.49 | | 3097.52 | | 3105.04 | | 3116.28 | | 3130.74 | | 3132.44 | | 3151.44 | | 3170.02 | | 3179.16 | | 3609.41 | | |  | | --- | | 1.5453 | | 1.2241 | | 5.8144 | | 0.5329 | | 1.6806 | | 3.9177 | | 5.7278 | | 0.0104 | | 0.0978 | | 0.0892 | | 0.4322 | | 44.1407 | | 41.5306 | | 42.1724 | | 58.6732 | | 3.9243 | | 30.3889 | | 0.4437 | | 1.1704 | | 1.9214 | | 2.2165 | | 0.9549 | | 0.8195 | | 1.0435 | | 1.7039 | | 0.7932 | | 1.0522 | | 0.0796 | | 0.3439 | | 4.1573 | | 1.8083 | | 1.5029 | | 22.9115 | | 4.8425 | | 4.3807 | | 114.0015 | | 4.0765 | | 0.4138 | | 0.2109 | | 4.1366 | | 1.1965 | | 0.3378 | | 2.3742 | | 1.2055 | | 0.6613 | | 2.2658 | | 0.0785 | | 0.4317 | | 0.202 | | 1.2759 | | 0.1761 | | 0.3763 | | 0.6806 | | 5.2306 | | 0.756 | | 0.4358 | | 7.1499 | | 0.2417 | | 0.3342 | | 14.6164 | | 4.3073 | | 2.1516 | | 11.711 | | 4.4804 | | 256.1781 | | 20.0173 | | 22.9476 | | 7.9398 | | 19.4837 | | 13.9358 | | 39.7169 | | 11.9807 | | 19.2275 | | 48.7384 | | 45.7013 | | 7.5596 | | 2.2648 | | 47.2067 | | 33.8499 | | 22.0342 | | 589.4182 | |

Table S7: B3LYP/cc-pVTZ cartesian coordinates and vibrational frequencies of van-der-Waals complexes (vdW), transition states (TS), and products of the reactions of atomic and molecular oxygen with JP-10; the vdW R2-O2H, vdW R4-O2H, and tsR4-O2H are obtained at the MP2/cc-pVDZ level.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **JP-10** | | | |  | | | |
| C | 0.221599 | -0.586778 | 0.787828 |  |  |  |  |
| C | 0.221599 | -0.586778 | -0.787828 |  |  |  |  |
| C | 0.221599 | 0.917698 | 1.132164 |  |  |  |  |
| C | 0.221599 | 0.917698 | -1.132164 |  |  |  |  |
| C | -0.640430 | 1.510860 | 0.000000 |  |  |  |  |
| C | 1.610944 | 1.491910 | 0.780878 |  |  |  |  |
| C | 1.610944 | 1.491910 | -0.780878 |  |  |  |  |
| C | -1.025973 | -1.391810 | 1.205692 |  |  |  |  |
| C | -1.025973 | -1.391810 | -1.205692 |  |  |  |  |
| C | -1.332464 | -2.291529 | 0.000000 |  |  |  |  |
| H | 1.116767 | -1.067916 | 1.185227 |  |  |  |  |
| H | 1.116767 | -1.067916 | -1.185227 |  |  |  |  |
| H | -0.101929 | 1.137231 | 2.149267 |  |  |  |  |
| H | -0.101929 | 1.137231 | -2.149267 |  |  |  |  |
| H | -1.670972 | 1.157614 | 0.000000 |  |  |  |  |
| H | -0.652613 | 2.601951 | 0.000000 |  |  |  |  |
| H | 2.418876 | 0.892255 | 1.201430 |  |  |  |  |
| H | 1.721563 | 2.504095 | 1.171744 |  |  |  |  |
| H | 1.721563 | 2.504095 | -1.171744 |  |  |  |  |
| H | 2.418876 | 0.892255 | -1.201430 |  |  |  |  |
| H | -1.869551 | -0.719955 | 1.384894 |  |  |  |  |
| H | -0.867295 | -1.953863 | 2.126671 |  |  |  |  |
| H | -0.867295 | -1.953863 | -2.126671 |  |  |  |  |
| H | -1.869551 | -0.719955 | -1.384894 |  |  |  |  |
| H | -0.660917 | -3.154606 | 0.000000 |  |  |  |  |
| H | -2.353016 | -2.676881 | 0 |  |  |  |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **R1** | | | | **R2** | | | |
| C | 0.356808 | 0.791831 | -0.530988 | C | -0.367857 | -0.853431 | -0.460482 |
| C | 0.306839 | -0.781831 | -0.511081 | C | -0.341184 | 0.739732 | -0.549712 |
| C | -0.909247 | 1.179987 | 0.296881 | C | 0.873855 | -1.094842 | 0.366479 |
| C | -0.950367 | -1.087387 | 0.336458 | C | 0.915189 | 1.110978 | 0.277478 |
| C | -0.928521 | 0.060642 | 1.365959 | C | 0.898150 | 0.026865 | 1.392021 |
| C | -2.099939 | 0.789000 | -0.524269 | C | 2.140895 | -0.885474 | -0.434481 |
| C | -2.198711 | -0.711808 | -0.499849 | C | 2.174627 | 0.690305 | -0.520471 |
| C | 1.723928 | 1.179859 | 0.070428 | C | -1.735623 | -1.205494 | 0.158285 |
| C | 1.657420 | -1.233391 | 0.082264 | C | -1.699702 | 1.204189 | 0.010152 |
| C | 2.609570 | -0.053165 | -0.161268 | C | -2.633182 | -0.002263 | -0.164079 |
| H | 0.277473 | 1.180997 | -1.545990 | H | -0.276890 | -1.304312 | -1.448923 |
| H | 0.194274 | -1.187244 | -1.517718 | H | -0.231081 | 1.070387 | -1.583457 |
| H | -0.975840 | -2.097827 | 0.742262 | H | 0.931206 | 2.149093 | 0.610262 |
| H | -0.050345 | 0.054299 | 2.010286 | H | 0.023426 | 0.075124 | 2.037162 |
| H | -1.820111 | 0.091397 | 1.992398 | H | 1.795616 | 0.039603 | 2.010162 |
| H | -2.609640 | 1.433385 | -1.225666 | H | 2.103959 | -1.357978 | -1.415330 |
| H | -3.117591 | -1.057909 | -0.008343 | H | 3.021517 | -1.262225 | 0.086782 |
| H | -2.192756 | -1.167349 | -1.495715 | H | 3.078576 | 1.085558 | -0.056182 |
| H | 1.630318 | 1.369333 | 1.142746 | H | 2.148392 | 1.049337 | -1.549613 |
| H | 2.130629 | 2.086527 | -0.378501 | H | -1.643581 | -1.320204 | 1.240408 |
| H | 2.014041 | -2.164103 | -0.360161 | H | -2.128945 | -2.145937 | -0.227922 |
| H | 1.560276 | -1.409704 | 1.156724 | H | -2.066351 | 2.100800 | -0.491105 |
| H | 2.961562 | -0.067230 | -1.196427 | H | -1.609675 | 1.447883 | 1.071824 |
| H | 3.492062 | -0.074574 | 0.479762 | H | -2.975105 | -0.060414 | -1.201185 |
| H | -0.901028 | 2.207591 | 0.657136 | H | -3.522067 | 0.049889 | 0.465979 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **R3** | | | | **R4** | | | |
| C | 0.357220 | 0.789040 | -0.493336 | C | 0.386982 | 0.745511 | -0.346332 |
| C | 0.357220 | -0.789040 | -0.493336 | C | 0.373830 | -0.771908 | -0.459568 |
| C | -0.884615 | 1.136071 | 0.364225 | C | -0.882722 | 1.142475 | 0.353113 |
| C | -0.884615 | -1.136071 | 0.364225 | C | -0.932601 | -1.131885 | 0.291198 |
| C | -0.889656 | 0.000000 | 1.351703 | C | -1.004469 | -0.029734 | 1.370591 |
| C | -2.149542 | 0.781904 | -0.472582 | C | -2.081289 | 0.833922 | -0.582121 |
| C | -2.149542 | -0.781904 | -0.472582 | C | -2.113919 | -0.726898 | -0.619452 |
| C | 1.718837 | 1.202758 | 0.098313 | C | 1.771233 | 1.247046 | -0.055594 |
| C | 1.718837 | -1.202758 | 0.098313 | C | 1.734374 | -1.182593 | 0.141857 |
| C | 2.637239 | 0.000000 | -0.155561 | C | 2.661917 | -0.006477 | -0.217693 |
| H | 0.250809 | 1.189074 | -1.502976 | H | 0.323691 | -1.125168 | -1.496125 |
| H | 0.250809 | -1.189074 | -1.502976 | H | -0.889255 | 2.147470 | 0.770822 |
| H | -0.886695 | 2.148385 | 0.763180 | H | -0.980092 | -2.160334 | 0.646722 |
| H | -0.886694 | -2.148385 | 0.763181 | H | -0.185759 | -0.060090 | 2.089497 |
| H | -1.356771 | 0.000000 | 2.326702 | H | -1.949387 | -0.027044 | 1.917823 |
| H | -2.101546 | 1.204921 | -1.477358 | H | -1.947358 | 1.275129 | -1.568627 |
| H | -3.048160 | 1.172421 | 0.004885 | H | -3.004351 | 1.236430 | -0.162412 |
| H | -3.048160 | -1.172421 | 0.004885 | H | -3.055338 | -1.107766 | -0.221885 |
| H | -2.101546 | -1.204922 | -1.477358 | H | -2.004011 | -1.123002 | -1.629252 |
| H | 1.620652 | 1.362626 | 1.175268 | H | 1.831302 | 1.635067 | 0.971050 |
| H | 2.097249 | 2.129779 | -0.334168 | H | 2.086103 | 2.070038 | -0.704088 |
| H | 2.097249 | -2.129779 | -0.334168 | H | 2.095703 | -2.139750 | -0.236205 |
| H | 1.620652 | -1.362626 | 1.175268 | H | 1.653818 | -1.271026 | 1.228535 |
| H | 2.976297 | 0.000000 | -1.195430 | H | 2.982869 | -0.097348 | -1.257985 |
| H | 3.527560 | 0.000000 | 0.474775 | H | 3.562062 | 0.030623 | 0.396137 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **R5** | | | | **R6** | | | |
| C | 0.354822 | 0.825549 | -0.527558 | C | 0.378264 | 0.788215 | -0.592492 |
| C | 0.398518 | -0.747160 | -0.568349 | C | 0.378264 | -0.788214 | -0.592493 |
| C | -0.875036 | 1.119032 | 0.379462 | C | -0.814966 | 1.129964 | 0.326439 |
| C | -0.826934 | -1.141531 | 0.283694 | C | -0.814967 | -1.129965 | 0.326436 |
| C | -0.822960 | -0.052455 | 1.375750 | C | -0.746245 | -0.000002 | 1.372604 |
| C | -2.145412 | 0.778215 | -0.425799 | C | -2.120891 | 0.780262 | -0.416516 |
| C | -2.107161 | -0.780851 | -0.500026 | C | -2.120892 | -0.780260 | -0.416518 |
| C | 1.692891 | 1.232101 | -0.018594 | C | 1.763975 | 1.241534 | -0.071369 |
| C | 1.768750 | -1.159745 | 0.021685 | C | 1.763974 | -1.241534 | -0.071369 |
| C | 2.661012 | 0.099699 | -0.024271 | C | 2.569660 | 0.000000 | 0.088275 |
| H | 0.171613 | 1.258958 | -1.519951 | H | 0.211684 | 1.187054 | -1.593210 |
| H | 0.298379 | -1.124448 | -1.586799 | H | 0.211685 | -1.187052 | -1.593212 |
| H | -0.871702 | 2.120148 | 0.807533 | H | -0.788334 | 2.148027 | 0.713501 |
| H | -0.801317 | -2.173347 | 0.633018 | H | -0.788336 | -2.148030 | 0.713494 |
| H | 0.073615 | -0.050865 | 1.994937 | H | 0.174143 | -0.000004 | 1.956924 |
| H | -1.696761 | -0.099638 | 2.027529 | H | -1.592580 | -0.000003 | 2.061282 |
| H | -2.144533 | 1.246699 | -1.410624 | H | -2.143788 | 1.201565 | -1.422132 |
| H | -3.038112 | 1.123638 | 0.096950 | H | -2.986955 | 1.172048 | 0.118245 |
| H | -2.986862 | -1.216972 | -0.025396 | H | -2.986957 | -1.172046 | 0.118240 |
| H | -2.075452 | -1.151923 | -1.525102 | H | -2.143788 | -1.201559 | -1.422136 |
| H | 1.979056 | 2.263338 | 0.140529 | H | 1.664983 | 1.785478 | 0.880045 |
| H | 2.207755 | -1.998306 | -0.519133 | H | 2.237746 | 1.955603 | -0.755016 |
| H | 1.647388 | -1.481567 | 1.057547 | H | 2.237744 | -1.955605 | -0.755014 |
| H | 3.265714 | 0.106438 | -0.945315 | H | 1.664980 | -1.785477 | 0.880046 |
| H | 3.380277 | 0.140731 | 0.798313 | H | 3.610716 | 0.000001 | 0.380962 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R1-OH** | | | | **vdW R2-OH** | | | |
| C | -0.772810 | -0.657213 | -0.692403 | C | 0.273851 | 0.423926 | -0.757221 |
| C | -1.019410 | 0.859983 | -0.354834 | C | 1.043481 | -0.895272 | -0.292165 |
| C | 0.648642 | -0.912862 | -0.094862 | C | -1.056529 | 0.195484 | -0.076934 |
| C | 0.272106 | 1.270509 | 0.388679 | C | -0.001553 | -1.614043 | 0.598023 |
| C | 0.621563 | -0.015376 | 1.164488 | C | -0.725898 | -0.417084 | 1.275696 |
| C | 1.608738 | -0.148799 | -0.958924 | C | -1.887978 | -0.861903 | -0.771596 |
| C | 1.424137 | 1.315865 | -0.645727 | C | -1.130254 | -2.166033 | -0.308156 |
| C | -1.936338 | -1.432605 | -0.039277 | C | 1.149336 | 1.600354 | -0.280725 |
| C | -2.324308 | 0.896014 | 0.466896 | C | 2.321732 | -0.395011 | 0.407607 |
| C | -3.062600 | -0.396545 | 0.089088 | C | 2.561466 | 1.010267 | -0.161615 |
| H | -0.770848 | -0.833952 | -1.768052 | H | 0.160592 | 0.453004 | -1.840705 |
| H | -1.141337 | 1.452805 | -1.262561 | H | 1.304806 | -1.513630 | -1.151724 |
| H | 0.175723 | 2.178962 | 0.980969 | H | -2.010427 | 1.915653 | 0.153441 |
| H | -0.135557 | -0.307968 | 1.889868 | H | 0.428925 | -2.357868 | 1.268121 |
| H | 1.586704 | 0.033014 | 1.667746 | H | -0.078905 | 0.189382 | 1.905051 |
| H | 1.974006 | -0.514306 | -1.910731 | H | -1.601854 | -0.718344 | 1.848857 |
| H | 2.324605 | 1.761112 | -0.205062 | H | -1.900634 | -0.744536 | -1.854034 |
| H | 1.185059 | 1.915315 | -1.529002 | H | -2.919725 | -0.867514 | -0.420465 |
| H | -1.648901 | -1.788689 | 0.952964 | H | -1.796232 | -2.820077 | 0.254608 |
| H | -2.226343 | -2.308201 | -0.620409 | H | -0.739735 | -2.736708 | -1.150619 |
| H | -2.912037 | 1.793057 | 0.270530 | H | 0.811268 | 1.957100 | 0.694086 |
| H | -2.100411 | 0.891002 | 1.536662 | H | 1.096323 | 2.449626 | -0.961174 |
| H | -3.562805 | -0.270976 | -0.874963 | H | 3.165061 | -1.067970 | 0.248903 |
| H | -3.825960 | -0.682015 | 0.813950 | H | 2.164100 | -0.331839 | 1.487216 |
| H | 0.878226 | -1.967343 | 0.049546 | H | 3.019226 | 0.937044 | -1.151907 |
| O | 4.250659 | -0.681646 | 0.513332 | H | 3.225736 | 1.614584 | 0.456925 |
| H | 3.436283 | -0.572466 | -0.036847 | O | -2.451806 | 2.794748 | 0.301992 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R3-OH** | | | | **vdW R4-OH** | | | |
| C | -0.923025 | 0.789747 | 0.528084 | C | 0.389887 | 0.318598 | 0.458269 |
| C | -0.923016 | -0.789583 | 0.528334 | C | 0.286425 | -0.491632 | -0.832623 |
| C | 0.529605 | 1.137831 | 0.088002 | C | -0.920893 | 0.153746 | 1.181134 |
| C | 0.529620 | -1.137790 | 0.088369 | C | -1.108701 | -1.146934 | -0.678421 |
| C | 0.808682 | -0.000132 | -0.860509 | C | -1.209594 | -1.340425 | 0.850235 |
| C | 1.472666 | 0.781470 | 1.264380 | C | -2.043210 | 0.847851 | 0.365997 |
| C | 1.472676 | -0.781033 | 1.264633 | C | -2.168784 | -0.046656 | -0.907322 |
| C | -2.048635 | 1.204540 | -0.439484 | C | 1.757830 | 0.164010 | 1.067663 |
| C | -2.048623 | -1.204694 | -0.439103 | C | 1.547684 | -1.381273 | -0.798337 |
| C | -2.999478 | -0.000086 | -0.469911 | C | 2.581000 | -0.530378 | -0.037756 |
| H | -1.118872 | 1.191483 | 1.523482 | H | 0.576047 | 2.230282 | -0.216202 |
| H | -1.118863 | -1.191005 | 1.523858 | H | 0.315381 | 0.129843 | -1.734202 |
| H | 0.645418 | 2.149171 | -0.295539 | H | -0.902743 | 0.420444 | 2.235852 |
| H | 0.645451 | -2.149253 | -0.294843 | H | -1.253925 | -2.036979 | -1.288689 |
| H | 0.592296 | -0.000306 | -1.921180 | H | -0.467066 | -2.024374 | 1.260772 |
| H | 2.858315 | -0.000202 | -1.287534 | H | -2.199305 | -1.662413 | 1.178729 |
| H | 1.119327 | 1.203949 | 2.205086 | H | -1.799293 | 1.882150 | 0.130641 |
| H | 2.475971 | 1.165849 | 1.084947 | H | -2.971938 | 0.850405 | 0.937375 |
| H | 2.475987 | -1.165457 | 1.085328 | H | -3.165499 | -0.482119 | -0.982652 |
| H | 1.119338 | -1.203209 | 2.205475 | H | -1.987609 | 0.509647 | -1.827049 |
| H | -1.643359 | 1.374232 | -1.440607 | H | 1.695920 | -0.469823 | 1.962842 |
| H | -2.539061 | 2.128795 | -0.133213 | H | 2.203529 | 1.105846 | 1.397959 |
| H | -2.539040 | -2.128855 | -0.132535 | H | 1.885102 | -1.671384 | -1.793491 |
| H | -1.643348 | -1.374702 | -1.440172 | H | 1.343749 | -2.300287 | -0.242827 |
| H | -3.630759 | 0.000053 | 0.422829 | H | 3.003794 | 0.222381 | -0.706647 |
| H | -3.663345 | -0.000226 | -1.335189 | H | 3.410329 | -1.116740 | 0.357268 |
| O | 3.842715 | -0.000242 | -1.385870 | O | 0.705457 | 3.141460 | -0.585339 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R5-OH** | | | | **vdW R6-OH** | | | |
| C | 0.000263 | -0.204620 | 1.048616 | C | 0.124857 | 0.241986 | 0.782553 |
| C | 0.302265 | -1.241672 | -0.095180 | C | 0.124164 | 0.207567 | -0.793329 |
| C | 0.777390 | 1.062675 | 0.586286 | C | -1.319409 | -0.172185 | 1.135305 |
| C | 1.247730 | -0.454323 | -1.026855 | C | -1.320431 | -0.220775 | -1.126335 |
| C | 0.665407 | 0.970953 | -0.946793 | C | -1.641121 | -1.193511 | 0.026150 |
| C | 2.280484 | 0.786618 | 0.795788 | C | -2.261901 | 0.990436 | 0.760073 |
| C | 2.601843 | -0.270060 | -0.308035 | C | -2.262410 | 0.957058 | -0.800475 |
| C | -1.487970 | -0.130462 | 1.122979 | C | 1.234000 | -0.731744 | 1.246385 |
| C | -1.068034 | -1.618958 | -0.705775 | C | 1.231868 | -0.786562 | -1.215284 |
| C | -2.125839 | -1.237982 | 0.349812 | C | 2.023799 | -1.051580 | 0.021402 |
| H | 0.399903 | -0.526444 | 2.018616 | H | 0.340317 | 1.242605 | 1.155671 |
| H | 0.795906 | -2.132248 | 0.295655 | H | 0.340169 | 1.190797 | -1.209865 |
| H | 0.425644 | 1.984819 | 1.046306 | H | -1.436564 | -0.520699 | 2.160880 |
| H | 1.333422 | -0.882952 | -2.024630 | H | -1.438952 | -0.612978 | -2.135847 |
| H | -0.354296 | 1.056434 | -1.319637 | H | -1.003992 | -2.078218 | 0.044829 |
| H | 1.281311 | 1.710695 | -1.460041 | H | -2.681619 | -1.521099 | 0.033641 |
| H | 2.496291 | 0.425204 | 1.801685 | H | -1.914496 | 1.943054 | 1.160709 |
| H | 2.861166 | 1.697399 | 0.646862 | H | -3.263385 | 0.818250 | 1.155670 |
| H | 3.358204 | 0.103647 | -0.998701 | H | -3.264214 | 0.768616 | -1.187756 |
| H | 2.975811 | -1.207679 | 0.104701 | H | -1.914988 | 1.891621 | -1.241580 |
| H | -2.337894 | 1.488424 | -0.044277 | H | 0.796973 | -1.649635 | 1.668517 |
| H | -2.000446 | 0.394610 | 1.921212 | H | 1.845496 | -0.312482 | 2.050522 |
| H | -1.117171 | -2.672898 | -0.978152 | H | 1.842209 | -0.403957 | -2.038469 |
| H | -1.244034 | -1.046793 | -1.617973 | H | 0.793328 | -1.722141 | -1.595189 |
| H | -2.328828 | -2.090347 | 1.016819 | H | 3.227865 | 0.678377 | -0.013078 |
| H | -3.091907 | -0.972347 | -0.087232 | H | 2.888687 | -1.703653 | 0.035098 |
| O | -2.826790 | 2.087183 | -0.655784 | O | 3.655333 | 1.568425 | -0.032803 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR1-OH** | | | | **tsR2-OH** | | | |
| C | -0.684089 | -0.703386 | -0.616337 | C | 0.331526 | 0.442619 | -0.731374 |
| C | -0.958984 | 0.834603 | -0.427124 | C | 0.872733 | -0.993399 | -0.322555 |
| C | 0.674291 | -0.904512 | 0.109609 | C | -1.023046 | 0.440877 | -0.032312 |
| C | 0.280553 | 1.312267 | 0.359347 | C | -0.264922 | -1.559740 | 0.560298 |
| C | 0.576788 | 0.104798 | 1.271023 | C | -0.773575 | -0.290671 | 1.288043 |
| C | 1.734756 | -0.241588 | -0.760640 | C | -2.012059 | -0.469710 | -0.754693 |
| C | 1.494421 | 1.269002 | -0.598647 | C | -1.474870 | -1.887625 | -0.346104 |
| C | -1.895102 | -1.429452 | 0.006931 | C | 1.393846 | 1.444216 | -0.237735 |
| C | -2.316600 | 0.928363 | 0.298526 | C | 2.224745 | -0.738143 | 0.372356 |
| C | -3.027030 | -0.392582 | -0.030110 | C | 2.689769 | 0.625422 | -0.157438 |
| H | -0.600127 | -0.969084 | -1.670830 | H | 0.207601 | 0.528806 | -1.810748 |
| H | -1.022134 | 1.347562 | -1.388008 | H | 1.019965 | -1.618808 | -1.203989 |
| H | 0.150530 | 2.271937 | 0.857315 | H | -1.500812 | 1.649109 | 0.129038 |
| H | -0.221593 | -0.118071 | 1.976706 | H | 0.044059 | -2.385892 | 1.199869 |
| H | 1.512602 | 0.198809 | 1.821171 | H | -0.030397 | 0.180877 | 1.926989 |
| H | 1.841097 | -0.620935 | -1.775786 | H | -1.681139 | -0.461384 | 1.865917 |
| H | 2.360352 | 1.761845 | -0.151373 | H | -2.010655 | -0.310434 | -1.832023 |
| H | 1.301723 | 1.763272 | -1.552241 | H | -3.028525 | -0.314460 | -0.395047 |
| H | -1.682270 | -1.703861 | 1.043006 | H | -2.233549 | -2.443653 | 0.204633 |
| H | -2.141573 | -2.350190 | -0.522147 | H | -1.189748 | -2.487236 | -1.210515 |
| H | -2.888188 | 1.805521 | -0.005688 | H | 1.129629 | 1.822417 | 0.751804 |
| H | -2.166822 | 1.005358 | 1.378408 | H | 1.473880 | 2.311013 | -0.892756 |
| H | -3.454741 | -0.344888 | -1.035195 | H | 2.941383 | -1.537303 | 0.180200 |
| H | -3.841741 | -0.624597 | 0.656857 | H | 2.090974 | -0.684718 | 1.455776 |
| H | 0.885155 | -1.939751 | 0.371519 | H | 3.119969 | 0.509260 | -1.155936 |
| O | 3.981481 | -0.705651 | 0.322641 | H | 3.450856 | 1.090995 | 0.469530 |
| H | 2.841851 | -0.502800 | -0.260298 | O | -1.948547 | 2.758541 | 0.310792 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR3-OH** | | | | **tsR4-OH** | | | |
| C | -0.840475 | -0.791620 | -0.551145 | C | 0.380817 | 0.519905 | 0.332603 |
| C | -0.840477 | 0.786740 | -0.558175 | C | 0.316396 | -0.508174 | -0.834191 |
| C | 0.600522 | -1.138254 | -0.091165 | C | -0.909509 | 0.298551 | 1.120995 |
| C | 0.600598 | 1.137423 | -0.101506 | C | -1.007210 | -1.250104 | -0.538720 |
| C | 0.860385 | 0.004029 | 0.884249 | C | -1.045494 | -1.241107 | 1.003570 |
| C | 1.568017 | -0.786425 | -1.243172 | C | -2.110092 | 0.766186 | 0.267261 |
| C | 1.567986 | 0.775023 | -1.250327 | C | -2.175973 | -0.298297 | -0.872695 |
| C | -1.988422 | -1.204466 | 0.391344 | C | 1.737820 | 0.364724 | 1.016465 |
| C | -1.988310 | 1.207901 | 0.380781 | C | 1.631061 | -1.308695 | -0.723658 |
| C | -2.938282 | 0.001820 | 0.398753 | C | 2.609889 | -0.350500 | -0.026606 |
| H | -1.016333 | -1.195830 | -1.549058 | H | 0.374165 | 1.651203 | -0.148962 |
| H | -1.016508 | 1.182059 | -1.559615 | H | 0.270959 | -0.015255 | -1.807238 |
| H | 0.709887 | -2.148360 | 0.298416 | H | -0.891416 | 0.707425 | 2.129539 |
| H | 0.710095 | 2.151020 | 0.278864 | H | -1.079329 | -2.225971 | -1.017053 |
| H | 0.339117 | 0.008374 | 1.838602 | H | -0.228535 | -1.790385 | 1.470248 |
| H | 2.102962 | 0.005699 | 1.259828 | H | -1.987619 | -1.608299 | 1.413025 |
| H | 1.236889 | -1.213201 | -2.189825 | H | -1.968109 | 1.777240 | -0.108544 |
| H | 2.566394 | -1.169047 | -1.036929 | H | -3.021613 | 0.756987 | 0.865152 |
| H | 2.566369 | 1.159566 | -1.047724 | H | -3.125518 | -0.834018 | -0.854735 |
| H | 1.236741 | 1.193078 | -2.200825 | H | -2.071622 | 0.144304 | -1.863363 |
| H | -1.608991 | -1.378390 | 1.401592 | H | 1.625411 | -0.258723 | 1.909963 |
| H | -2.473732 | -2.126995 | 0.072181 | H | 2.153234 | 1.317226 | 1.345959 |
| H | -2.473539 | 2.127677 | 0.053650 | H | 1.989039 | -1.650862 | -1.694636 |
| H | -1.608765 | 1.390528 | 1.389444 | H | 1.480552 | -2.196940 | -0.104588 |
| H | -3.551738 | -0.002116 | -0.506276 | H | 2.992968 | 0.377922 | -0.744801 |
| H | -3.619416 | 0.005579 | 1.250385 | H | 3.468281 | -0.859308 | 0.412444 |
| O | 3.286415 | 0.007166 | 1.586185 | O | 0.431614 | 2.844065 | -0.709070 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR5-OH** | | | | **tsR6-OH** | | | |
| C | -0.141546 | -0.013232 | 0.995418 | C | 0.116043 | 0.787808 | -0.261506 |
| C | 0.110400 | -1.220595 | 0.017834 | C | 0.116052 | -0.787840 | -0.261303 |
| C | 0.820266 | 1.076382 | 0.460971 | C | -1.305058 | 1.131923 | 0.232088 |
| C | 1.197700 | -0.671969 | -0.929761 | C | -1.305032 | -1.131855 | 0.232404 |
| C | 0.799108 | 0.811585 | -1.057003 | C | -1.581426 | 0.000170 | 1.241958 |
| C | 2.258747 | 0.646981 | 0.818970 | C | -2.302098 | 0.780538 | -0.892590 |
| C | 2.518070 | -0.560736 | -0.136779 | C | -2.302082 | -0.780822 | -0.892377 |
| C | -1.639728 | 0.255379 | 0.932400 | C | 1.278020 | 1.215526 | 0.659048 |
| C | -1.258769 | -1.537743 | -0.620749 | C | 1.278005 | -1.215318 | 0.659368 |
| C | -2.298006 | -0.990719 | 0.369509 | C | 2.180872 | 0.000111 | 0.749377 |
| H | 0.118175 | -0.258148 | 2.029336 | H | 0.283494 | 1.182594 | -1.263143 |
| H | 0.475648 | -2.095413 | 0.558098 | H | 0.283495 | -1.182884 | -1.262839 |
| H | 0.561564 | 2.084798 | 0.777465 | H | -1.406126 | 2.149369 | 0.608513 |
| H | 1.288076 | -1.228403 | -1.861829 | H | -1.406063 | -2.149199 | 0.609114 |
| H | -0.174039 | 0.972983 | -1.520611 | H | -0.908732 | 0.000293 | 2.099800 |
| H | 1.536367 | 1.406518 | -1.597882 | H | -2.607029 | 0.000209 | 1.613708 |
| H | 2.359449 | 0.380782 | 1.871624 | H | -1.999926 | 1.201117 | -1.851968 |
| H | 2.959455 | 1.458787 | 0.622319 | H | -3.294196 | 1.171739 | -0.665025 |
| H | 3.354525 | -0.357193 | -0.805912 | H | -3.294172 | -1.171984 | -0.664713 |
| H | 2.750446 | -1.480491 | 0.401158 | H | -1.999890 | -1.201657 | -1.851637 |
| H | -1.846134 | 1.160738 | 0.102932 | H | 0.911778 | 1.456412 | 1.664230 |
| H | -2.088391 | 0.686968 | 1.826443 | H | 1.795915 | 2.105412 | 0.299605 |
| H | -1.386261 | -2.602028 | -0.817567 | H | 1.795892 | -2.105317 | 0.300197 |
| H | -1.363171 | -1.019348 | -1.575788 | H | 0.911727 | -1.455897 | 1.664612 |
| H | -2.459976 | -1.705134 | 1.185774 | H | 2.867379 | -0.000034 | -0.288136 |
| H | -3.271696 | -0.797377 | -0.081143 | H | 2.941121 | 0.000206 | 1.529326 |
| O | -2.126435 | 2.077495 | -0.777411 | O | 3.510695 | -0.000229 | -1.417556 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R1-O2H** | | | | **vdW R2-O2H** | | | |
| C | -0.507452 | -0.708164 | 0.321538 | C | -0.043276 | 0.434461 | -0.505791 |
| C | -1.057497 | 0.138299 | -0.886946 | C | 1.524169 | 0.152366 | -0.527007 |
| C | 0.173582 | 0.370962 | 1.215553 | C | -0.506924 | -0.764630 | 0.301938 |
| C | -0.661835 | 1.585133 | -0.513900 | C | 1.663893 | -1.151591 | 0.298297 |
| C | -0.793229 | 1.572269 | 1.022573 | C | 0.556036 | -0.970806 | 1.375816 |
| C | 1.377584 | 0.877793 | 0.470581 | C | -0.471955 | -2.047167 | -0.513372 |
| C | 0.870275 | 1.730960 | -0.669368 | C | 1.080190 | -2.322193 | -0.534678 |
| C | -1.730262 | -1.427786 | 0.925665 | C | -0.199768 | 1.829624 | 0.135655 |
| C | -2.570047 | -0.160204 | -0.949303 | C | 2.167090 | 1.415425 | 0.085417 |
| C | -2.735631 | -1.507922 | -0.232117 | C | 1.135881 | 2.526741 | -0.166945 |
| H | 0.220882 | -1.449330 | -0.006086 | H | -0.480677 | 0.423418 | -1.517080 |
| H | -0.585253 | -0.156492 | -1.825026 | H | 1.883981 | 0.001416 | -1.560441 |
| H | -1.231453 | 2.349139 | -1.040204 | H | -2.229504 | -0.219789 | 0.652761 |
| H | -1.802794 | 1.374668 | 1.379937 | H | 2.685201 | -1.332722 | 0.673759 |
| H | -0.432158 | 2.487665 | 1.491678 | H | 0.716442 | -0.105221 | 2.036456 |
| H | 1.183543 | 2.773638 | -0.543350 | H | 0.399384 | -1.877273 | 1.983914 |
| H | 1.231311 | 1.419018 | -1.654161 | H | -0.902078 | -1.914620 | -1.518351 |
| H | -2.156406 | -0.841845 | 1.743635 | H | -1.009560 | -2.867527 | -0.009296 |
| H | -1.471917 | -2.404634 | 1.334577 | H | 1.310815 | -3.291663 | -0.061602 |
| H | -2.947036 | -0.174414 | -1.972125 | H | 1.487342 | -2.339907 | -1.559497 |
| H | -3.131009 | 0.610980 | -0.414892 | H | -0.327955 | 1.736766 | 1.229960 |
| H | -2.460977 | -2.324037 | -0.905559 | H | -1.080513 | 2.363245 | -0.254820 |
| H | -3.757526 | -1.693638 | 0.100446 | H | 3.158655 | 1.629448 | -0.347699 |
| H | 0.362450 | 0.048288 | 2.236959 | H | 2.304465 | 1.282051 | 1.174682 |
| H | 2.348749 | 1.022533 | 0.930683 | H | 1.165233 | 2.827377 | -1.230920 |
| O | 4.182935 | -0.957603 | 0.035916 | H | 1.306740 | 3.430271 | 0.442432 |
| O | 3.071306 | -1.208722 | -0.634159 | O | -3.318509 | 0.545029 | -0.609785 |
| H | 2.402742 | -0.538975 | -0.296214 | O | -3.158989 | 0.160140 | 0.631006 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R3-O2H** | | | | **vdW R4-O2H** | | | |
| C | 0.708905 | 1.027648 | 0.788596 | C | 0.369232 | -0.123234 | 0.648194 |
| C | 0.708905 | 1.027648 | -0.788596 | C | 0.301841 | -0.427834 | -0.857101 |
| C | -0.757361 | 0.684935 | 1.138550 | C | -0.959654 | -0.540218 | 1.238432 |
| C | -0.757361 | 0.684935 | -1.138550 | C | -1.094994 | -1.081618 | -0.975105 |
| C | -1.155265 | -0.223373 | 0.000000 | C | -1.229387 | -1.811717 | 0.381154 |
| C | -1.632611 | 1.923427 | 0.782384 | C | -2.062176 | 0.407999 | 0.701205 |
| C | -1.632611 | 1.923427 | -0.782384 | C | -2.141727 | 0.047145 | -0.817046 |
| C | 1.772024 | -0.008460 | 1.204902 | C | 1.723133 | -0.527584 | 1.195050 |
| C | 1.772024 | -0.008460 | -1.204902 | C | 1.557369 | -1.296980 | -1.089974 |
| C | 2.718018 | -0.101909 | 0.000000 | C | 2.571450 | -0.731165 | -0.077649 |
| H | 0.972233 | 2.008243 | 1.186685 | H | 0.498062 | 1.717812 | 0.565156 |
| H | 0.972233 | 2.008243 | -1.186685 | H | 0.362109 | 0.484020 | -1.480358 |
| H | -0.909171 | 0.313321 | 2.149423 | H | -0.959989 | -0.674011 | 2.331619 |
| H | -0.909171 | 0.313321 | -2.149423 | H | -1.228696 | -1.698523 | -1.878723 |
| H | -0.472640 | -1.906370 | 0.000000 | H | -0.480515 | -2.607002 | 0.536819 |
| H | -2.076459 | -0.801631 | 0.000000 | H | -2.238133 | -2.228924 | 0.551291 |
| H | -1.218187 | 2.838379 | 1.207084 | H | -1.818786 | 1.467810 | 0.875398 |
| H | -2.642910 | 1.807588 | 1.173362 | H | -3.017105 | 0.195412 | 1.211288 |
| H | -2.642910 | 1.807588 | -1.173362 | H | -3.148602 | -0.316270 | -1.083522 |
| H | -1.218187 | 2.838379 | -1.207084 | H | -1.909935 | 0.909624 | -1.462874 |
| H | 1.307147 | -0.981881 | 1.381246 | H | 1.619847 | -1.483835 | 1.749693 |
| H | 2.282055 | 0.269309 | 2.127640 | H | 2.154326 | 0.203070 | 1.902806 |
| H | 2.282055 | 0.269309 | -2.127640 | H | 1.913667 | -1.259419 | -2.132774 |
| H | 1.307147 | -0.981881 | -1.381246 | H | 1.339097 | -2.353033 | -0.843752 |
| H | 3.407688 | 0.746600 | 0.000000 | H | 2.938792 | 0.248464 | -0.434674 |
| H | 3.321456 | -1.009919 | 0.000000 | H | 3.446225 | -1.382881 | 0.082533 |
| O | -0.296075 | -2.909153 | 0.000000 | O | 0.583738 | 2.713608 | 0.455240 |
| O | -1.482722 | -3.480537 | 0.000000 | O | 0.206151 | 2.947507 | -0.776852 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **vdW R5-O2H** | | | | **vdW R6-O2H** | | | |
| C | -0.265931 | 0.180784 | 0.982522 | C | 0.102029 | -0.542138 | 0.411286 |
| C | -1.104927 | 1.184990 | 0.109529 | C | 0.309471 | 0.487352 | -0.764462 |
| C | -0.605528 | -1.201198 | 0.351366 | C | 1.526335 | -0.698270 | 0.984972 |
| C | -1.848639 | 0.248632 | -0.866123 | C | 1.824216 | 0.777248 | -0.703880 |
| C | -0.792096 | -0.841466 | -1.134071 | C | 2.101805 | 0.721369 | 0.811617 |
| C | -2.051133 | -1.553800 | 0.757963 | C | 2.372120 | -1.494315 | -0.030818 |
| C | -2.907630 | -0.545005 | -0.070830 | C | 2.576737 | -0.476575 | -1.196570 |
| C | 1.143234 | 0.669213 | 0.896101 | C | -0.942047 | 0.080163 | 1.366855 |
| C | -0.081942 | 2.146112 | -0.540054 | C | -0.613965 | 1.691076 | -0.465058 |
| C | 1.197109 | 2.045147 | 0.314343 | C | -1.533070 | 1.233419 | 0.621867 |
| H | -0.581883 | 0.174348 | 2.032879 | H | -0.271224 | -1.496908 | 0.042797 |
| H | -1.811179 | 1.748516 | 0.720262 | H | 0.041044 | 0.051692 | -1.726666 |
| H | 0.122962 | -1.977952 | 0.576416 | H | 1.548669 | -1.108368 | 1.993950 |
| H | -2.246458 | 0.758553 | -1.742618 | H | 2.115175 | 1.694612 | -1.214595 |
| H | 0.112215 | -0.471340 | -1.616298 | H | 1.573160 | 1.483617 | 1.384812 |
| H | -1.177244 | -1.672883 | -1.725466 | H | 3.163174 | 0.786270 | 1.054876 |
| H | -2.210510 | -1.460203 | 1.832432 | H | 1.871088 | -2.407670 | -0.352092 |
| H | -2.284330 | -2.583008 | 0.484166 | H | 3.327550 | -1.785382 | 0.406700 |
| H | -3.585004 | -1.068983 | -0.745522 | H | 3.634691 | -0.257926 | -1.344552 |
| H | -3.516565 | 0.104993 | 0.558277 | H | 2.185410 | -0.840624 | -2.146876 |
| H | 2.224761 | -0.404771 | -0.295186 | H | -0.467650 | 0.437393 | 2.293436 |
| H | 1.921138 | 0.290967 | 1.552895 | H | -1.693545 | -0.647111 | 1.684819 |
| H | -0.460019 | 3.166229 | -0.599357 | H | -1.143453 | 2.044186 | -1.354197 |
| H | 0.136016 | 1.830361 | -1.561869 | H | -0.029113 | 2.556024 | -0.117443 |
| H | 1.175848 | 2.787626 | 1.126884 | H | -2.869887 | 0.305674 | -0.283227 |
| H | 2.111928 | 2.251365 | -0.246447 | H | -2.252550 | 1.903429 | 1.080916 |
| O | 2.925179 | -0.932384 | -0.781539 | O | -3.576674 | -0.240775 | -0.758740 |
| O | 3.821474 | -1.251899 | 0.137049 | O | -3.557618 | -1.433585 | -0.193449 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR1-O2H** | | | | **tsR2-O2H** | | | |
| C | -0.495616 | -0.721972 | 0.281931 | C | -0.033601 | -0.457722 | -0.577851 |
| C | -1.050496 | 0.182051 | -0.881492 | C | -1.548604 | 0.018249 | -0.475686 |
| C | 0.235132 | 0.300902 | 1.197450 | C | 0.642594 | 0.658162 | 0.201858 |
| C | -0.600814 | 1.601054 | -0.468777 | C | -1.460242 | 1.314773 | 0.367472 |
| C | -0.695605 | 1.539558 | 1.069280 | C | -0.306707 | 0.979534 | 1.354403 |
| C | 1.448394 | 0.807421 | 0.454666 | C | 0.700697 | 1.950431 | -0.601831 |
| C | 0.930320 | 1.705855 | -0.656832 | C | -0.799653 | 2.416804 | -0.499795 |
| C | -1.723725 | -1.428222 | 0.890681 | C | -0.004059 | -1.871197 | 0.040796 |
| C | -2.572515 | -0.068935 | -0.914223 | C | -2.297082 | -1.164603 | 0.176234 |
| C | -2.759882 | -1.436883 | -0.242466 | C | -1.435565 | -2.391804 | -0.161264 |
| H | 0.202670 | -1.470198 | -0.090442 | H | 0.323843 | -0.484011 | -1.620163 |
| H | -0.611268 | -0.093384 | -1.841171 | H | -1.964904 | 0.230724 | -1.476594 |
| H | -1.157865 | 2.400414 | -0.954728 | H | 2.022283 | 0.132363 | 0.537187 |
| H | -1.701305 | 1.360388 | 1.446882 | H | -2.418865 | 1.615394 | 0.822939 |
| H | -0.294474 | 2.426675 | 1.559906 | H | -0.522603 | 0.129512 | 2.019525 |
| H | 1.278851 | 2.733233 | -0.512092 | H | 0.009483 | 1.848655 | 1.955191 |
| H | 1.257647 | 1.404729 | -1.655742 | H | 1.032916 | 1.780371 | -1.637938 |
| H | -2.112476 | -0.861387 | 1.740257 | H | 1.376052 | 2.687946 | -0.136952 |
| H | -1.484230 | -2.426528 | 1.257053 | H | -0.869122 | 3.399300 | -0.003097 |
| H | -2.975917 | -0.033778 | -1.926419 | H | -1.279181 | 2.502891 | -1.489214 |
| H | -3.095946 | 0.697841 | -0.337034 | H | 0.219144 | -1.810994 | 1.121941 |
| H | -2.526383 | -2.234983 | -0.952031 | H | 0.772581 | -2.502171 | -0.418744 |
| H | -3.778102 | -1.605474 | 0.109862 | H | -3.337505 | -1.245873 | -0.180873 |
| H | 0.432815 | -0.062976 | 2.203247 | H | -2.334183 | -1.032296 | 1.273629 |
| H | 2.362047 | 1.060083 | 0.986568 | H | -1.583734 | -2.670667 | -1.221273 |
| O | 4.059961 | -1.049384 | -0.037079 | H | -1.671622 | -3.275911 | 0.454796 |
| O | 2.895433 | -1.171758 | -0.614016 | O | 3.190166 | -0.931244 | -0.495426 |
| H | 2.269621 | -0.410494 | -0.206676 | O | 2.994677 | -0.321381 | 0.627129 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR3-O2H** | | | | **tsR4-O2H** | | | |
| C | 0.752162 | 0.978413 | 0.788471 | C | 0.359874 | -0.027627 | 0.619729 |
| C | 0.752162 | 0.978413 | -0.788471 | C | 0.276664 | -0.440477 | -0.864324 |
| C | -0.728701 | 0.708246 | 1.138575 | C | -0.983137 | -0.379265 | 1.236379 |
| C | -0.728701 | 0.708246 | -1.138575 | C | -1.135100 | -1.066756 | -0.933677 |
| C | -1.175437 | -0.179715 | 0.000000 | C | -1.277344 | -1.700476 | 0.469204 |
| C | -1.542086 | 1.987998 | 0.782436 | C | -2.070070 | 0.548782 | 0.639713 |
| C | -1.542086 | 1.987998 | -0.782436 | C | -2.157655 | 0.091258 | -0.851442 |
| C | 1.765533 | -0.106447 | 1.205086 | C | 1.683493 | -0.508327 | 1.195575 |
| C | 1.765533 | -0.106447 | -1.205086 | C | 1.503649 | -1.359690 | -1.052092 |
| C | 2.706073 | -0.243658 | 0.000000 | C | 2.532966 | -0.790663 | -0.058381 |
| H | 1.062252 | 1.945438 | 1.186081 | H | 0.509983 | 1.428784 | 0.552775 |
| H | 1.062252 | 1.945438 | -1.186081 | H | 0.356776 | 0.432550 | -1.538805 |
| H | -0.898791 | 0.344851 | 2.149556 | H | -0.981402 | -0.437824 | 2.336372 |
| H | -0.898791 | 0.344851 | -2.149556 | H | -1.284100 | -1.741095 | -1.792896 |
| H | -0.586732 | -1.793564 | 0.000000 | H | -0.542904 | -2.497568 | 0.675314 |
| H | -2.143664 | -0.677107 | 0.000000 | H | -2.292465 | -2.085995 | 0.672740 |
| H | -1.083026 | 2.881350 | 1.207158 | H | -1.810286 | 1.613437 | 0.745078 |
| H | -2.556847 | 1.922115 | 1.173472 | H | -3.026981 | 0.382705 | 1.162871 |
| H | -2.556847 | 1.922115 | -1.173472 | H | -3.172024 | -0.267051 | -1.095553 |
| H | -1.083026 | 2.881350 | -1.207158 | H | -1.907020 | 0.904108 | -1.552443 |
| H | 1.256571 | -1.057251 | 1.381720 | H | 1.509585 | -1.445931 | 1.762807 |
| H | 2.288164 | 0.147996 | 2.127507 | H | 2.144757 | 0.210202 | 1.895891 |
| H | 2.288164 | 0.147996 | -2.127507 | H | 1.864052 | -1.375858 | -2.093939 |
| H | 1.256571 | -1.057251 | -1.381720 | H | 1.248627 | -2.397373 | -0.766030 |
| H | 3.434435 | 0.571888 | 0.000000 | H | 2.936337 | 0.161136 | -0.449986 |
| H | 3.266444 | -1.178833 | 0.000000 | H | 3.382523 | -1.466718 | 0.133969 |
| O | -0.422969 | -2.817981 | 0.000000 | O | 0.652874 | 2.518676 | 0.429818 |
| O | -1.608760 | -3.378228 | 0.000000 | O | 0.430188 | 2.779065 | -0.811350 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **tsR5-O2H** | | | | **tsR6-O2H** | | | |
| C | 0.237001 | -0.165886 | 0.984433 | C | 0.098941 | -0.585726 | 0.358764 |
| C | 0.969975 | -1.220224 | 0.075475 | C | 0.302567 | 0.527286 | -0.738603 |
| C | 0.694150 | 1.192704 | 0.381485 | C | 1.517324 | -0.754457 | 0.943354 |
| C | 1.783905 | -0.333088 | -0.889514 | C | 1.810240 | 0.841123 | -0.633807 |
| C | 0.829756 | 0.856133 | -1.115513 | C | 2.067074 | 0.684239 | 0.878301 |
| C | 2.171206 | 1.399905 | 0.775661 | C | 2.393694 | -1.461265 | -0.111810 |
| C | 2.921516 | 0.339256 | -0.090720 | C | 2.594684 | -0.360841 | -1.200641 |
| C | -1.220301 | -0.527853 | 0.919366 | C | -0.972117 | -0.051434 | 1.336303 |
| C | -0.146177 | -2.070928 | -0.571204 | C | -0.649199 | 1.687262 | -0.368551 |
| C | -1.373116 | -1.907047 | 0.343658 | C | -1.599032 | 1.122391 | 0.646093 |
| H | 0.564294 | -0.217023 | 2.029175 | H | -0.248954 | -1.519519 | -0.081510 |
| H | 1.629372 | -1.859500 | 0.664017 | H | 0.056310 | 0.155625 | -1.733065 |
| H | 0.043711 | 2.027790 | 0.634382 | H | 1.533235 | -1.233538 | 1.921596 |
| H | 2.121870 | -0.855482 | -1.783590 | H | 2.090380 | 1.797365 | -1.074471 |
| H | -0.109695 | 0.587432 | -1.596200 | H | 1.515634 | 1.394393 | 1.495135 |
| H | 1.285362 | 1.664539 | -1.688616 | H | 3.123389 | 0.751659 | 1.142014 |
| H | 2.334879 | 1.264121 | 1.845017 | H | 1.916054 | -2.359422 | -0.503783 |
| H | 2.494650 | 2.410236 | 0.524242 | H | 3.348359 | -1.763750 | 0.319594 |
| H | 3.635131 | 0.817063 | -0.762330 | H | 3.650078 | -0.112489 | -1.316459 |
| H | 3.476834 | -0.379505 | 0.512726 | H | 2.224228 | -0.664932 | -2.179933 |
| H | -2.002689 | 0.416096 | -0.089305 | H | -0.518659 | 0.275782 | 2.283325 |
| H | -1.901004 | -0.184747 | 1.695956 | H | -1.702280 | -0.818381 | 1.606907 |
| H | 0.147864 | -3.113433 | -0.689001 | H | -1.153854 | 2.110896 | -1.240409 |
| H | -0.381410 | -1.693227 | -1.568028 | H | -0.091699 | 2.522696 | 0.079180 |
| H | -1.341793 | -2.642375 | 1.160833 | H | -2.741548 | 0.354887 | -0.227435 |
| H | -2.324931 | -2.067218 | -0.166864 | H | -2.290318 | 1.771699 | 1.176007 |
| O | -2.648219 | 1.022840 | -0.702810 | O | -3.472964 | -0.185555 | -0.778342 |
| O | -3.711774 | 1.283086 | 0.002664 | O | -3.538963 | -1.383750 | -0.262046 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **JP-10** | |  |  |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 132.37 | 0.0112 |  |  |
| ν2 | 175.83 | 0.0024 |  |  |
| ν3 | 264.43 | 0.0613 |  |  |
| ν4 | 314.4 | 0.0388 |  |  |
| ν5 | 316.61 | 0.0535 |  |  |
| ν6 | 394.96 | 0.0293 |  |  |
| ν7 | 489.18 | 0.2313 |  |  |
| ν8 | 532.92 | 0.1785 |  |  |
| ν9 | 554.31 | 0.6264 |  |  |
| ν10 | 671.91 | 0.6036 |  |  |
| ν11 | 738.15 | 0.2999 |  |  |
| ν12 | 752.67 | 0.3414 |  |  |
| ν13 | 791.27 | 1.3181 |  |  |
| ν14 | 829.07 | 0.5855 |  |  |
| ν15 | 864.53 | 1.0142 |  |  |
| ν16 | 865.08 | 0.0232 |  |  |
| ν17 | 887.77 | 0.5934 |  |  |
| ν18 | 891.04 | 0.0758 |  |  |
| ν19 | 912.58 | 0.8196 |  |  |
| ν20 | 917.25 | 0.0674 |  |  |
| ν21 | 923.99 | 0.9959 |  |  |
| ν22 | 955.67 | 1.8485 |  |  |
| ν23 | 961.26 | 0.0214 |  |  |
| ν24 | 990.79 | 1.6513 |  |  |
| ν25 | 998.36 | 0.5391 |  |  |
| ν26 | 1042.02 | 0.2663 |  |  |
| ν27 | 1048.92 | 0.4814 |  |  |
| ν28 | 1052.57 | 0.0513 |  |  |
| ν29 | 1053.46 | 0.025 |  |  |
| ν30 | 1073.39 | 0.6124 |  |  |
| ν31 | 1137.02 | 0.1158 |  |  |
| ν32 | 1151.23 | 0.0064 |  |  |
| ν33 | 1169.34 | 1.0532 |  |  |
| ν34 | 1194.09 | 0.198 |  |  |
| ν35 | 1203.91 | 0.0851 |  |  |
| ν36 | 1207.67 | 1.4543 |  |  |
| ν37 | 1226.44 | 1.2542 |  |  |
| ν38 | 1253.48 | 0.0104 |  |  |
| ν39 | 1262.65 | 0.7486 |  |  |
| ν40 | 1292.21 | 1.2505 |  |  |
| ν41 | 1305.31 | 0.0002 |  |  |
| ν42 | 1307.75 | 0.2664 |  |  |
| ν43 | 1314.54 | 0.4983 |  |  |
| ν44 | 1320.92 | 0.0042 |  |  |
| ν45 | 1326.65 | 0.0641 |  |  |
| ν46 | 1333.18 | 1.0454 |  |  |
| ν47 | 1344.57 | 0.7653 |  |  |
| ν48 | 1352.54 | 0.9778 |  |  |
| ν49 | 1367.11 | 0.8201 |  |  |
| ν50 | 1371.99 | 0.4778 |  |  |
| ν51 | 1493.72 | 0.1473 |  |  |
| ν52 | 1495.36 | 2.3993 |  |  |
| ν53 | 1496.43 | 1.1264 |  |  |
| ν54 | 1502.51 | 6.5608 |  |  |
| ν55 | 1513.53 | 8.926 |  |  |
| ν56 | 1524.14 | 3.8204 |  |  |
| ν57 | 3016.21 | 16.8227 |  |  |
| ν58 | 3021.07 | 29.0278 |  |  |
| ν59 | 3024.72 | 24.1971 |  |  |
| ν60 | 3029.55 | 1.3904 |  |  |
| ν61 | 3034.93 | 24.4597 |  |  |
| ν62 | 3042.89 | 17.3718 |  |  |
| ν63 | 3044.74 | 82.9402 |  |  |
| ν64 | 3046.88 | 34.4594 |  |  |
| ν65 | 3063 | 5.8434 |  |  |
| ν66 | 3067.74 | 45.6645 |  |  |
| ν67 | 3070.4 | 31.8506 |  |  |
| ν68 | 3072.12 | 109.9999 |  |  |
| ν69 | 3076.4 | 45.4314 |  |  |
| ν70 | 3079.32 | 11.4533 |  |  |
| ν71 | 3085.88 | 99.6687 |  |  |
| ν72 | 3090.62 | 39.6989 |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R1** | | **R2** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 144.14 | 0.0916 | 137.73 | 0.0767 |
| ν2 | 172.45 | 0.1305 | 173.99 | 0.0496 |
| ν3 | 267.5 | 7.2001 | 266.86 | 0.2483 |
| ν4 | 298 | 2.165 | 313.65 | 0.2096 |
| ν5 | 315.87 | 0.3488 | 316.41 | 0.2939 |
| ν6 | 366.1 | 5.5818 | 394.46 | 0.0744 |
| ν7 | 435.92 | 13.0759 | 492.3 | 0.599 |
| ν8 | 491.93 | 0.4299 | 522.52 | 0.7427 |
| ν9 | 547.4 | 0.0591 | 552.08 | 0.618 |
| ν10 | 566.54 | 3.3887 | 664.62 | 1.1613 |
| ν11 | 671.19 | 0.5024 | 713.45 | 0.1548 |
| ν12 | 743.93 | 0.6185 | 749.37 | 0.269 |
| ν13 | 763.34 | 0.2909 | 769.77 | 0.6977 |
| ν14 | 791.79 | 1.5729 | 824.04 | 0.4542 |
| ν15 | 861.88 | 0.2907 | 834.7 | 3.756 |
| ν16 | 863.91 | 0.3945 | 853.7 | 0.4236 |
| ν17 | 886.39 | 0.5003 | 871.01 | 0.181 |
| ν18 | 900.77 | 1.2501 | 882.7 | 0.3417 |
| ν19 | 907.54 | 0.486 | 908.99 | 1.6557 |
| ν20 | 912.59 | 0.8491 | 915.2 | 0.2637 |
| ν21 | 932.46 | 0.1256 | 928.22 | 1.3881 |
| ν22 | 935.22 | 0.2481 | 947.59 | 1.3123 |
| ν23 | 955.54 | 2.0572 | 966.65 | 0.5089 |
| ν24 | 978.33 | 0.7943 | 991.39 | 0.7622 |
| ν25 | 994.17 | 1.0163 | 1002.8 | 1.6883 |
| ν26 | 1008.42 | 1.4141 | 1037.72 | 0.4684 |
| ν27 | 1032.36 | 0.0319 | 1048.55 | 0.1456 |
| ν28 | 1040.72 | 0.7618 | 1059.42 | 0.1583 |
| ν29 | 1049.02 | 0.026 | 1083.87 | 0.1635 |
| ν30 | 1069.1 | 0.6036 | 1093.98 | 0.1091 |
| ν31 | 1119.32 | 0.4389 | 1140.49 | 1.0979 |
| ν32 | 1142.62 | 0.2572 | 1163.29 | 0.1783 |
| ν33 | 1154.7 | 0.6472 | 1190.06 | 0.1626 |
| ν34 | 1184.65 | 0.7262 | 1196.93 | 0.6595 |
| ν35 | 1193.68 | 0.3631 | 1207.64 | 4.6767 |
| ν36 | 1207.11 | 0.1274 | 1217.27 | 1.3779 |
| ν37 | 1231.32 | 1.2258 | 1233.13 | 1.5708 |
| ν38 | 1251.86 | 0.8086 | 1255.58 | 0.9227 |
| ν39 | 1272.11 | 0.402 | 1262.96 | 0.6151 |
| ν40 | 1283.04 | 1.9516 | 1292 | 1.6531 |
| ν41 | 1302.23 | 0.1749 | 1301.77 | 0.6656 |
| ν42 | 1306.89 | 0.1404 | 1308.57 | 0.2938 |
| ν43 | 1319.51 | 0.3661 | 1315.41 | 0.7123 |
| ν44 | 1324.17 | 0.3823 | 1321.25 | 1.0947 |
| ν45 | 1336.03 | 1.3279 | 1335.26 | 0.4959 |
| ν46 | 1343.25 | 0.9062 | 1343.39 | 0.3136 |
| ν47 | 1345.69 | 0.5726 | 1358.6 | 0.4468 |
| ν48 | 1359.53 | 1.1246 | 1372.6 | 0.762 |
| ν49 | 1366.83 | 0.4175 | 1490.52 | 1.0101 |
| ν50 | 1473.74 | 3.8526 | 1492.99 | 0.0972 |
| ν51 | 1494.17 | 1.621 | 1496.24 | 2.5589 |
| ν52 | 1495.91 | 2.5165 | 1500.85 | 7.364 |
| ν53 | 1505.73 | 5.1738 | 1511.11 | 6.8655 |
| ν54 | 1518.41 | 7.6693 | 1522.39 | 5.5066 |
| ν55 | 2962.7 | 47.8864 | 3017.6 | 23.3304 |
| ν56 | 3005.25 | 27.6022 | 3024.99 | 27.5936 |
| ν57 | 3017.44 | 18.3495 | 3034.22 | 16.5652 |
| ν58 | 3023.01 | 31.5333 | 3036.72 | 13.5793 |
| ν59 | 3026.27 | 24.7536 | 3038.81 | 18.3207 |
| ν60 | 3036.08 | 8.3388 | 3047.68 | 47.047 |
| ν61 | 3051.88 | 48.6339 | 3052.82 | 49.4094 |
| ν62 | 3053.71 | 10.7873 | 3057.79 | 27.5609 |
| ν63 | 3067.94 | 38.65 | 3067.8 | 42.5488 |
| ν64 | 3072.11 | 42.4071 | 3071.04 | 33.7399 |
| ν65 | 3078.2 | 81.4318 | 3073.07 | 56.3947 |
| ν66 | 3079.83 | 96.0844 | 3074.57 | 13.1348 |
| ν67 | 3083.68 | 6.6638 | 3083.2 | 53.6511 |
| ν68 | 3096.52 | 33.3638 | 3094.52 | 74.4557 |
| ν69 | 3192.55 | 22.4166 | 3108.19 | 32.335 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R3** | | **R4** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 112.75 | 0.0013 | 118.71 | 0.0982 |
| ν2 | 178.4 | 0.1225 | 156.58 | 0.1601 |
| ν3 | 251.42 | 0.037 | 234.82 | 0.4595 |
| ν4 | 300.12 | 1.3246 | 281.27 | 0.2846 |
| ν5 | 314.22 | 0.0548 | 314.04 | 0.0844 |
| ν6 | 333.29 | 8.0965 | 383.13 | 0.0241 |
| ν7 | 423.63 | 5.0365 | 482.08 | 0.6028 |
| ν8 | 532.05 | 0.5301 | 538.75 | 0.2116 |
| ν9 | 544.12 | 0.9831 | 560.16 | 1.0979 |
| ν10 | 665.9 | 13.1529 | 620.83 | 3.3064 |
| ν11 | 671.51 | 0.2193 | 719.6 | 0.077 |
| ν12 | 737.38 | 1.3347 | 737.1 | 0.2361 |
| ν13 | 762.63 | 0.6053 | 795.28 | 1.9847 |
| ν14 | 791.98 | 0.8512 | 825.7 | 0.7923 |
| ν15 | 831.42 | 1.563 | 843.08 | 0.17 |
| ν16 | 850.8 | 0.3443 | 872.27 | 0.7838 |
| ν17 | 867.47 | 0.0807 | 878.75 | 0.5798 |
| ν18 | 872.88 | 1.1343 | 886.89 | 0.3659 |
| ν19 | 909 | 0.0569 | 891.39 | 0.6118 |
| ν20 | 915.01 | 1.9186 | 903.4 | 0.2422 |
| ν21 | 921.14 | 0.0378 | 915.97 | 0.8334 |
| ν22 | 947.82 | 1.3689 | 954.23 | 0.079 |
| ν23 | 947.98 | 0.134 | 957.47 | 2.9678 |
| ν24 | 987.98 | 1.5697 | 987.35 | 1.1165 |
| ν25 | 990.03 | 0.0979 | 1014.5 | 0.2568 |
| ν26 | 992.66 | 0.997 | 1036.96 | 0.0286 |
| ν27 | 1036.21 | 0.1587 | 1043.09 | 1.0385 |
| ν28 | 1048.32 | 0.092 | 1058.67 | 0.1445 |
| ν29 | 1055.38 | 0.1271 | 1090.39 | 1.1632 |
| ν30 | 1072.28 | 0.6894 | 1122.98 | 0.4735 |
| ν31 | 1152.62 | 0.3515 | 1131.23 | 0.137 |
| ν32 | 1163.64 | 1.0785 | 1148.93 | 0.1773 |
| ν33 | 1187.04 | 0.9747 | 1165.15 | 0.6424 |
| ν34 | 1191.49 | 0.2726 | 1189.63 | 1.8604 |
| ν35 | 1203.2 | 0.3981 | 1205.61 | 1.3702 |
| ν36 | 1205.53 | 0.3846 | 1221.96 | 1.0038 |
| ν37 | 1237.15 | 1.1689 | 1230.18 | 0.3143 |
| ν38 | 1246.11 | 0.0073 | 1249.07 | 0.3255 |
| ν39 | 1260.48 | 1.5996 | 1252.11 | 0.5066 |
| ν40 | 1277.88 | 0.0043 | 1285.64 | 1.1026 |
| ν41 | 1301.24 | 0.0147 | 1303.8 | 0.6094 |
| ν42 | 1308.16 | 0.3664 | 1309.86 | 0.2144 |
| ν43 | 1316.38 | 0.007 | 1312.03 | 0.1984 |
| ν44 | 1328.09 | 0.1424 | 1324.56 | 1.122 |
| ν45 | 1332.26 | 0.4739 | 1337.28 | 0.5783 |
| ν46 | 1345.31 | 0.5263 | 1341.01 | 1.2093 |
| ν47 | 1346.75 | 0.3768 | 1350.3 | 0.0196 |
| ν48 | 1363.3 | 2.1732 | 1363.06 | 0.3218 |
| ν49 | 1366.74 | 0.4244 | 1474.48 | 3.1552 |
| ν50 | 1489.61 | 3.0274 | 1491.73 | 0.3539 |
| ν51 | 1492.68 | 0.6336 | 1493.77 | 1.4779 |
| ν52 | 1494.24 | 5.2637 | 1499.83 | 5.8859 |
| ν53 | 1508.07 | 0.7402 | 1507.59 | 7.0511 |
| ν54 | 1509.95 | 6.5107 | 1520.41 | 2.1935 |
| ν55 | 3014.87 | 20.9594 | 2955.29 | 36.2429 |
| ν56 | 3020.93 | 32.1861 | 2976.34 | 27.4842 |
| ν57 | 3024.68 | 22.8561 | 3011.5 | 21.9143 |
| ν58 | 3029.64 | 7.1275 | 3023.08 | 14.2887 |
| ν59 | 3033.54 | 28.0222 | 3033.31 | 52.8643 |
| ν60 | 3041.28 | 15.2047 | 3036.15 | 26.4074 |
| ν61 | 3046.42 | 88.4567 | 3036.66 | 41.546 |
| ν62 | 3065.25 | 0.0936 | 3047.21 | 64.4467 |
| ν63 | 3067.92 | 38.5508 | 3069.7 | 13.186 |
| ν64 | 3070.38 | 50.0545 | 3070.4 | 54.6294 |
| ν65 | 3077.91 | 61.4707 | 3079.35 | 61.0943 |
| ν66 | 3086.04 | 65.1896 | 3079.7 | 37.7455 |
| ν67 | 3090.49 | 74.4246 | 3084.8 | 44.56 |
| ν68 | 3093.56 | 14.3785 | 3090.44 | 22.6704 |
| ν69 | 3185.75 | 18.6547 | 3093.15 | 61.0325 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **R5** | | **R6** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 117.54 | 0.078 | 44.39 | 0.9717 |
| ν2 | 130.03 | 0.2488 | 105.48 | 0.001 |
| ν3 | 260.81 | 0.2589 | 256.3 | 0.017 |
| ν4 | 278.81 | 0.4121 | 257.55 | 0.7199 |
| ν5 | 314.66 | 0.4143 | 323.58 | 0 |
| ν6 | 393.11 | 0.5897 | 389.9 | 17.5186 |
| ν7 | 423.72 | 19.2794 | 395.34 | 6.8536 |
| ν8 | 497.02 | 1.0396 | 494.33 | 0.1102 |
| ν9 | 534 | 0.1252 | 527.9 | 0.0025 |
| ν10 | 627.67 | 0.5817 | 693.96 | 0.3037 |
| ν11 | 737.25 | 0.0973 | 718.94 | 0.4832 |
| ν12 | 749.56 | 1.4282 | 729.5 | 0.1642 |
| ν13 | 765.25 | 0.9295 | 764.56 | 0.0285 |
| ν14 | 795.78 | 0.7469 | 796.61 | 1.0192 |
| ν15 | 830.66 | 0.3578 | 829.04 | 0.7482 |
| ν16 | 845.15 | 0.4212 | 835.9 | 0.4135 |
| ν17 | 869.45 | 0.9338 | 887.43 | 0.4564 |
| ν18 | 886.7 | 0.658 | 889.07 | 0.812 |
| ν19 | 904.13 | 0.2894 | 908.77 | 0.7099 |
| ν20 | 921.91 | 0.0814 | 924.6 | 1.0064 |
| ν21 | 924.93 | 1.3023 | 936.59 | 0.4479 |
| ν22 | 947.98 | 1.3356 | 941.94 | 0.9111 |
| ν23 | 960.55 | 0.1525 | 962.31 | 0.0613 |
| ν24 | 977.33 | 1.585 | 964.3 | 1.2647 |
| ν25 | 1000.35 | 0.8711 | 1012.62 | 1.6014 |
| ν26 | 1018.04 | 0.38 | 1019.76 | 0.0168 |
| ν27 | 1046.88 | 0.4199 | 1043.6 | 0.5475 |
| ν28 | 1050.01 | 0.1124 | 1055.13 | 0.7413 |
| ν29 | 1063.81 | 0.3506 | 1059.14 | 0.3877 |
| ν30 | 1073.9 | 1.1094 | 1082.78 | 0.0481 |
| ν31 | 1118.89 | 0.0402 | 1127.43 | 0.478 |
| ν32 | 1141.4 | 0.2253 | 1139.44 | 0.6212 |
| ν33 | 1159.52 | 0.7048 | 1146.52 | 0.1233 |
| ν34 | 1183.37 | 0.2825 | 1174.32 | 0.6634 |
| ν35 | 1206.14 | 2.6552 | 1199.12 | 0.0617 |
| ν36 | 1217 | 0.8212 | 1210.9 | 1.252 |
| ν37 | 1229.67 | 0.5063 | 1230.86 | 1.4038 |
| ν38 | 1246.93 | 0.0596 | 1251.82 | 0.0033 |
| ν39 | 1278.47 | 0.3802 | 1267.67 | 0.0054 |
| ν40 | 1286.32 | 1.0909 | 1293.03 | 1.0358 |
| ν41 | 1295.15 | 0.122 | 1301.71 | 0.1589 |
| ν42 | 1299.97 | 0.3742 | 1305.94 | 0.1114 |
| ν43 | 1311.11 | 0.3983 | 1309.85 | 0.4764 |
| ν44 | 1319.79 | 0.968 | 1322.05 | 0.3622 |
| ν45 | 1322.92 | 1.3454 | 1328.56 | 2.0577 |
| ν46 | 1334.76 | 2.2571 | 1347.86 | 0.085 |
| ν47 | 1348.15 | 0.7248 | 1354.3 | 2.4838 |
| ν48 | 1361.49 | 1.0143 | 1364.48 | 0.0572 |
| ν49 | 1370.92 | 1.212 | 1377.57 | 1.3146 |
| ν50 | 1472.81 | 1.8999 | 1471.5 | 5.5625 |
| ν51 | 1494.92 | 1.0556 | 1474.42 | 1.8097 |
| ν52 | 1496.09 | 3.1172 | 1494.93 | 1.0178 |
| ν53 | 1507.38 | 10.2599 | 1503.57 | 8.3837 |
| ν54 | 1520.71 | 2.8065 | 1522.32 | 3.4532 |
| ν55 | 2915.82 | 48.3636 | 2932.28 | 37.7165 |
| ν56 | 2948.9 | 37.5495 | 2934.23 | 29.0825 |
| ν57 | 3022.4 | 28.5809 | 2983.45 | 37.9977 |
| ν58 | 3034.74 | 26.2904 | 2983.63 | 26.3922 |
| ν59 | 3040.46 | 24.6668 | 3034.46 | 20.1696 |
| ν60 | 3043.34 | 20.5903 | 3043.05 | 46.2238 |
| ν61 | 3044.25 | 74.3395 | 3044.88 | 17.4481 |
| ν62 | 3046.6 | 30.0892 | 3045.28 | 45.6163 |
| ν63 | 3062.85 | 4.5672 | 3060.42 | 53.313 |
| ν64 | 3074.43 | 62.3167 | 3063.07 | 9.496 |
| ν65 | 3077.52 | 56.994 | 3073.14 | 86.2422 |
| ν66 | 3083.26 | 25.8908 | 3079.75 | 4.2022 |
| ν67 | 3086.63 | 73.6727 | 3084.8 | 46.3141 |
| ν68 | 3090.17 | 31.1567 | 3086.94 | 69.297 |
| ν69 | 3173.89 | 24.6839 | 3179.57 | 31.2055 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW R1-OH** | | **vdW R2-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 34.67 | 2.2341 | 29.5 | 1.6018 |
| ν2 | 49.18 | 2.7602 | 33.41 | 1.9271 |
| ν3 | 110.54 | 0.3226 | 117.35 | 0.0673 |
| ν4 | 147.99 | 0.7535 | 136.44 | 0.0516 |
| ν5 | 178.8 | 0.5656 | 174.92 | 0.0433 |
| ν6 | 292.87 | 1.1954 | 265.13 | 0.3102 |
| ν7 | 314.18 | 0.9586 | 312.68 | 0.1121 |
| ν8 | 320.57 | 2.5221 | 315.88 | 0.1015 |
| ν9 | 388.71 | 0.4457 | 394.28 | 0.0995 |
| ν10 | 476.03 | 60.2942 | 489.65 | 3.2687 |
| ν11 | 489.42 | 36.4313 | 513.19 | 25.0076 |
| ν12 | 499.34 | 29.1939 | 537.77 | 40.8873 |
| ν13 | 542.39 | 35.179 | 549.79 | 29.0164 |
| ν14 | 552.08 | 4.7228 | 556 | 29.8317 |
| ν15 | 618.08 | 31.9418 | 662.57 | 1.2422 |
| ν16 | 671.79 | 0.5105 | 710.26 | 0.3886 |
| ν17 | 743.73 | 1.5346 | 749.83 | 0.2754 |
| ν18 | 766.09 | 0.3978 | 770.46 | 0.9756 |
| ν19 | 793.9 | 1.7245 | 825.14 | 0.7536 |
| ν20 | 861 | 1.6552 | 837.86 | 1.5367 |
| ν21 | 863.48 | 0.3244 | 855.16 | 0.5558 |
| ν22 | 887.56 | 0.591 | 870.69 | 0.3188 |
| ν23 | 901.62 | 1.2749 | 884.07 | 0.3658 |
| ν24 | 907.25 | 0.4466 | 909.19 | 1.7766 |
| ν25 | 912.21 | 0.4658 | 914.52 | 0.1815 |
| ν26 | 931.41 | 0.3592 | 930 | 1.448 |
| ν27 | 933.55 | 0.3333 | 949.06 | 0.7645 |
| ν28 | 954.94 | 3.9593 | 968.1 | 0.2518 |
| ν29 | 980.61 | 0.7543 | 991.2 | 0.7287 |
| ν30 | 998.21 | 1.6943 | 1003.84 | 1.7231 |
| ν31 | 1009.34 | 1.6054 | 1037.64 | 0.5651 |
| ν32 | 1032.76 | 0.0488 | 1048.3 | 0.1524 |
| ν33 | 1041.18 | 1.0015 | 1061.28 | 0.1915 |
| ν34 | 1049.8 | 0.0157 | 1084.85 | 0.2919 |
| ν35 | 1073.16 | 1.7395 | 1094.16 | 0.1141 |
| ν36 | 1126.29 | 0.8699 | 1142.1 | 1.8982 |
| ν37 | 1147.79 | 0.1996 | 1165.49 | 1.0857 |
| ν38 | 1156.86 | 0.777 | 1191.36 | 0.3022 |
| ν39 | 1185.42 | 0.5803 | 1198.09 | 0.9587 |
| ν40 | 1194.79 | 0.3792 | 1207.56 | 6.0398 |
| ν41 | 1207.92 | 0.2427 | 1219.36 | 1.4835 |
| ν42 | 1232.08 | 1.5779 | 1236.19 | 1.8953 |
| ν43 | 1253.23 | 1.0518 | 1256.96 | 0.9031 |
| ν44 | 1272.75 | 0.3841 | 1263.91 | 0.424 |
| ν45 | 1285.66 | 2.3056 | 1293.21 | 2.069 |
| ν46 | 1302.57 | 0.2267 | 1302.32 | 1.0444 |
| ν47 | 1308.45 | 0.4104 | 1310.44 | 0.3604 |
| ν48 | 1320.84 | 0.6729 | 1317.12 | 0.5485 |
| ν49 | 1325.59 | 0.6556 | 1323.45 | 0.9846 |
| ν50 | 1334.04 | 1.8021 | 1336.73 | 0.5393 |
| ν51 | 1343.37 | 0.7713 | 1344.22 | 0.314 |
| ν52 | 1346.71 | 0.4965 | 1359.45 | 0.632 |
| ν53 | 1360.97 | 1.2283 | 1374.18 | 0.3956 |
| ν54 | 1368.12 | 0.6324 | 1491.14 | 1.3246 |
| ν55 | 1469 | 5.1656 | 1493.64 | 0.23 |
| ν56 | 1495.34 | 1.9362 | 1495.39 | 2.7309 |
| ν57 | 1496.68 | 2.804 | 1501.61 | 7.6312 |
| ν58 | 1507.89 | 3.3919 | 1511.24 | 6.4151 |
| ν59 | 1522.33 | 9.5702 | 1523.31 | 6.9196 |
| ν60 | 2977.92 | 30.7494 | 3019.74 | 21.4966 |
| ν61 | 3019.46 | 19.1784 | 3027.02 | 27.6727 |
| ν62 | 3023.32 | 14.6018 | 3039.54 | 13.3643 |
| ν63 | 3025.67 | 31.3902 | 3041.82 | 7.3922 |
| ν64 | 3029.54 | 24.3785 | 3044.53 | 22.649 |
| ν65 | 3037.12 | 8.4382 | 3054.15 | 32.5557 |
| ν66 | 3052.33 | 37.4339 | 3058.96 | 42.6635 |
| ν67 | 3062.04 | 11.9571 | 3064.53 | 17.7147 |
| ν68 | 3071.04 | 38.6185 | 3072.64 | 30.0775 |
| ν69 | 3075.12 | 41.8223 | 3076.27 | 48.2444 |
| ν70 | 3082.76 | 75.6567 | 3077.27 | 48.0084 |
| ν71 | 3082.98 | 69.6326 | 3081.03 | 11.4474 |
| ν72 | 3087.83 | 10.1442 | 3089.09 | 47.5226 |
| ν73 | 3106.56 | 24.638 | 3101.57 | 57.0882 |
| ν74 | 3162.29 | 20.1079 | 3116.67 | 26.0955 |
| ν75 | 3386.25 | 299.2574 | 3243.95 | 297.4061 |
|  | **vdW R3-OH** | | **vdW R4-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 31.96 | 1.9521 | 33.58 | 1.6595 |
| ν2 | 51.24 | 2.627 | 49.67 | 2.363 |
| ν3 | 102.34 | 0.1827 | 116.68 | 0.0735 |
| ν4 | 117.05 | 0.2951 | 124.83 | 0.1713 |
| ν5 | 184.08 | 0.7473 | 167.07 | 0.6637 |
| ν6 | 257.78 | 0.0129 | 249.65 | 1.196 |
| ν7 | 309.33 | 0.8064 | 284.58 | 0.3864 |
| ν8 | 314.58 | 0.1619 | 314.04 | 0.5603 |
| ν9 | 391.74 | 2.6605 | 385.75 | 0.0127 |
| ν10 | 426.24 | 9.925 | 484.43 | 0.7529 |
| ν11 | 452.62 | 54.6468 | 515.3 | 58.2087 |
| ν12 | 506.86 | 86.4264 | 531.36 | 29.4202 |
| ν13 | 531.47 | 0.2534 | 548.53 | 41.024 |
| ν14 | 553.1 | 2.0794 | 558.26 | 1.9571 |
| ν15 | 664.35 | 1.8755 | 636.23 | 5.0957 |
| ν16 | 717.92 | 12.7592 | 719.4 | 0.1844 |
| ν17 | 740.53 | 0.5144 | 738.18 | 0.5997 |
| ν18 | 766.2 | 12.6196 | 793.6 | 2.3261 |
| ν19 | 789.45 | 0.8442 | 827.39 | 1.0255 |
| ν20 | 840.48 | 2.5554 | 847.23 | 0.1073 |
| ν21 | 846.05 | 0.6727 | 872.92 | 0.8435 |
| ν22 | 867.19 | 0.5757 | 877.67 | 0.9114 |
| ν23 | 883.39 | 0.9571 | 887.11 | 0.5044 |
| ν24 | 893.08 | 0.804 | 893.91 | 0.4327 |
| ν25 | 914.53 | 0.0446 | 903.92 | 0.08 |
| ν26 | 914.65 | 2.2032 | 916.92 | 0.8357 |
| ν27 | 943.14 | 1.4322 | 955.09 | 0.9419 |
| ν28 | 980.9 | 0.4579 | 958.24 | 2.4491 |
| ν29 | 982.74 | 1.4369 | 988.9 | 1.1862 |
| ν30 | 985.12 | 0.0233 | 1014.62 | 0.4707 |
| ν31 | 1010.62 | 0.9248 | 1038.58 | 0.0252 |
| ν32 | 1035.86 | 0.4501 | 1045.09 | 1.2739 |
| ν33 | 1045.36 | 0.1284 | 1059.48 | 0.0296 |
| ν34 | 1056.27 | 0.1295 | 1087.59 | 1.1826 |
| ν35 | 1072.79 | 0.7356 | 1122.81 | 0.2192 |
| ν36 | 1151.31 | 1.0893 | 1134.46 | 0.2442 |
| ν37 | 1171.35 | 1.8807 | 1154.85 | 0.6179 |
| ν38 | 1180.95 | 0.6504 | 1163.01 | 1.027 |
| ν39 | 1192.01 | 0.4109 | 1187.1 | 2.6156 |
| ν40 | 1201.91 | 0.3459 | 1205.6 | 1.6855 |
| ν41 | 1217.08 | 0.2159 | 1223.6 | 1.4885 |
| ν42 | 1234.72 | 0.1017 | 1231.16 | 0.2773 |
| ν43 | 1253.37 | 2.2294 | 1250.68 | 0.2709 |
| ν44 | 1260.49 | 0.9991 | 1254.25 | 1.1011 |
| ν45 | 1275.92 | 0.1441 | 1286.71 | 1.1869 |
| ν46 | 1301.5 | 0.0205 | 1303.46 | 0.2171 |
| ν47 | 1305.51 | 0.4978 | 1310.4 | 0.2546 |
| ν48 | 1317.15 | 0.1382 | 1313.08 | 0.0976 |
| ν49 | 1327.21 | 0.241 | 1326.43 | 1.3336 |
| ν50 | 1334.73 | 0.5237 | 1340.01 | 0.6236 |
| ν51 | 1344.52 | 0.6845 | 1341.49 | 0.5137 |
| ν52 | 1344.88 | 0.4008 | 1350.04 | 0.4063 |
| ν53 | 1360.96 | 0.2253 | 1358.03 | 0.3873 |
| ν54 | 1365.76 | 2.5 | 1470.22 | 6.5338 |
| ν55 | 1475.63 | 0.0938 | 1492.38 | 0.8626 |
| ν56 | 1493.92 | 2.8922 | 1497.97 | 1.7781 |
| ν57 | 1496.33 | 5.1057 | 1501.44 | 5.4227 |
| ν58 | 1510.91 | 2.7605 | 1508.57 | 8.0771 |
| ν59 | 1514.85 | 7.0096 | 1522.89 | 2.4138 |
| ν60 | 3017.49 | 13.9449 | 2964.96 | 26.208 |
| ν61 | 3020.97 | 28.8017 | 2987.99 | 17.0751 |
| ν62 | 3026.64 | 31.4963 | 3024.59 | 21.394 |
| ν63 | 3032.42 | 0.0662 | 3027.62 | 3.4462 |
| ν64 | 3043.82 | 31.5081 | 3040.08 | 40.4197 |
| ν65 | 3045.44 | 22.3587 | 3041.84 | 27.6185 |
| ν66 | 3054.7 | 64.9224 | 3042.55 | 35.6 |
| ν67 | 3071.91 | 38.2749 | 3052.44 | 51.1791 |
| ν68 | 3074.3 | 30.9074 | 3075.86 | 3.4809 |
| ν69 | 3075.53 | 15.3445 | 3077.12 | 58.084 |
| ν70 | 3081.37 | 60.0786 | 3083.84 | 59.7234 |
| ν71 | 3095.09 | 62.2718 | 3085.3 | 25.8482 |
| ν72 | 3095.56 | 18.4366 | 3089.08 | 39.1889 |
| ν73 | 3099.19 | 33.1865 | 3094.7 | 24.5872 |
| ν74 | 3169.4 | 13.605 | 3100.58 | 36.8133 |
| ν75 | 3372.37 | 275.5598 | 3324.28 | 281.8576 |
|  | **vdW R5-OH** | | **vdW R6-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 31.84 | 1.7789 | 29.17 | 2.2935 |
| ν2 | 48.34 | 1.8513 | 31.16 | 2.3311 |
| ν3 | 95.14 | 0.2494 | 98.34 | 0.2037 |
| ν4 | 132.81 | 0.2407 | 119.72 | 0.1593 |
| ν5 | 159.09 | 2.5202 | 172.36 | 5.4222 |
| ν6 | 264.03 | 0.2642 | 258 | 0.2089 |
| ν7 | 296.12 | 1.736 | 274.79 | 1.2496 |
| ν8 | 315.19 | 1.4068 | 320.35 | 1.0875 |
| ν9 | 394.75 | 1.1806 | 393.65 | 4.338 |
| ν10 | 431.82 | 85.1826 | 441.63 | 56.5173 |
| ν11 | 438.28 | 59.2958 | 452.62 | 47.1751 |
| ν12 | 495.22 | 11.1572 | 489.47 | 10.2232 |
| ν13 | 533.15 | 6.5314 | 533.41 | 0.0637 |
| ν14 | 541.69 | 21.7777 | 534.42 | 62.0755 |
| ν15 | 636.4 | 3.8224 | 691.22 | 1.6782 |
| ν16 | 737.16 | 0.2874 | 691.5 | 1.3417 |
| ν17 | 746.34 | 0.96 | 731.46 | 0.2608 |
| ν18 | 775.61 | 2.856 | 775.96 | 0.4837 |
| ν19 | 797.64 | 0.4546 | 796.32 | 0.6349 |
| ν20 | 829.98 | 0.3954 | 828.32 | 0.7722 |
| ν21 | 848.68 | 0.3419 | 844.53 | 0.6844 |
| ν22 | 869.84 | 1.7206 | 886.48 | 0.5198 |
| ν23 | 887.03 | 0.6403 | 888.23 | 0.4033 |
| ν24 | 903.65 | 0.2831 | 912.2 | 0.6834 |
| ν25 | 920.65 | 0.4237 | 923.44 | 1.1716 |
| ν26 | 924.38 | 1.4443 | 927.01 | 0.7851 |
| ν27 | 947.71 | 1.0358 | 950.21 | 1.2157 |
| ν28 | 960.99 | 0.1207 | 961.99 | 0.0178 |
| ν29 | 980.49 | 1.177 | 965.07 | 1.1607 |
| ν30 | 998.75 | 1.0993 | 1007.23 | 3.8437 |
| ν31 | 1016.82 | 1.0084 | 1023.74 | 0.0027 |
| ν32 | 1046 | 0.1423 | 1043.88 | 0.6649 |
| ν33 | 1050.24 | 0.1047 | 1052.74 | 0.5806 |
| ν34 | 1060.42 | 0.8123 | 1058.12 | 0.3018 |
| ν35 | 1071.54 | 1.821 | 1068.42 | 0.4481 |
| ν36 | 1122.22 | 0.203 | 1129.98 | 0.7868 |
| ν37 | 1143.88 | 0.4023 | 1145.37 | 0.0085 |
| ν38 | 1161.3 | 0.5363 | 1150.8 | 1.0968 |
| ν39 | 1184.8 | 1.1546 | 1182.97 | 0.4464 |
| ν40 | 1204.93 | 2.8879 | 1196.81 | 0.1123 |
| ν41 | 1217.82 | 0.4363 | 1211.93 | 1.3274 |
| ν42 | 1227.86 | 0.3336 | 1232.95 | 1.6353 |
| ν43 | 1247.74 | 0.1595 | 1249.9 | 0.1381 |
| ν44 | 1277.56 | 0.8224 | 1263.47 | 0.5344 |
| ν45 | 1288.37 | 1.4109 | 1292.83 | 0.8666 |
| ν46 | 1295.44 | 1.4265 | 1307.18 | 0.0641 |
| ν47 | 1300.99 | 0.3541 | 1307.58 | 0.1685 |
| ν48 | 1313.69 | 0.6619 | 1307.69 | 0.1179 |
| ν49 | 1318.98 | 1.3908 | 1322.19 | 0.7117 |
| ν50 | 1323.81 | 0.1712 | 1326.87 | 2.7391 |
| ν51 | 1335.53 | 2.5229 | 1343.71 | 0.0073 |
| ν52 | 1348.64 | 1.7499 | 1353.14 | 3.22 |
| ν53 | 1362.39 | 0.5999 | 1366.28 | 0.0893 |
| ν54 | 1368.95 | 0.9293 | 1373.46 | 0.6594 |
| ν55 | 1468.43 | 5.5208 | 1463.06 | 5.0912 |
| ν56 | 1495.16 | 1.2143 | 1471.13 | 2.7258 |
| ν57 | 1498.47 | 2.1661 | 1495.65 | 1.0964 |
| ν58 | 1508.6 | 12.202 | 1504.23 | 9.7094 |
| ν59 | 1523.49 | 2.7833 | 1523.12 | 3.7739 |
| ν60 | 2929.3 | 32.48 | 2932.18 | 16.6271 |
| ν61 | 2963.89 | 28.3246 | 2934.89 | 27.634 |
| ν62 | 3029.3 | 16.1912 | 3018.03 | 28.1619 |
| ν63 | 3037.41 | 24.8631 | 3019.06 | 16.7718 |
| ν64 | 3045.16 | 21.156 | 3037.45 | 19.9857 |
| ν65 | 3045.5 | 6.9261 | 3044.5 | 39.0211 |
| ν66 | 3047.78 | 94.6336 | 3047.81 | 49.3061 |
| ν67 | 3050.2 | 12.5271 | 3053.62 | 16.5938 |
| ν68 | 3065.7 | 4.1386 | 3066.9 | 15.2941 |
| ν69 | 3078.25 | 69.9068 | 3069.02 | 33.317 |
| ν70 | 3082.63 | 24.9538 | 3074.01 | 80.3611 |
| ν71 | 3085.14 | 18.7127 | 3081.54 | 2.2359 |
| ν72 | 3088.8 | 80.0611 | 3084.64 | 33.2568 |
| ν73 | 3093.58 | 32.2448 | 3089.31 | 81.8036 |
| ν74 | 3149.72 | 21.6937 | 3160.63 | 27.4172 |
| ν75 | 3456.42 | 189.3358 | 3411.42 | 236.6912 |
|  | **tsR1-OH** | | **tsR2-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -932.5 | 891.971 | -1274.16 | 562.6168 |
| ν2 | 70.7 | 2.332 | 72.87 | 2.411 |
| ν3 | 78.81 | 2.6707 | 84.1 | 1.767 |
| ν4 | 146.04 | 0.7486 | 144.95 | 0.2605 |
| ν5 | 178.37 | 0.6195 | 175.14 | 0.0211 |
| ν6 | 269.32 | 4.9218 | 268.37 | 0.2518 |
| ν7 | 306.58 | 1.2243 | 309.06 | 0.5869 |
| ν8 | 322.16 | 0.7114 | 316.56 | 0.1363 |
| ν9 | 375.06 | 1.143 | 377.68 | 2.2338 |
| ν10 | 493.41 | 0.3357 | 398.88 | 0.6269 |
| ν11 | 539.95 | 3.519 | 490.43 | 0.1806 |
| ν12 | 558.36 | 1.3247 | 530.84 | 1.2352 |
| ν13 | 631.8 | 82.1758 | 553.38 | 0.9572 |
| ν14 | 681.26 | 24.3216 | 666.82 | 0.9409 |
| ν15 | 746.63 | 11.746 | 722.66 | 1.147 |
| ν16 | 757.58 | 2.9913 | 753.34 | 1.8528 |
| ν17 | 794.22 | 1.5093 | 790.7 | 3.2541 |
| ν18 | 842.54 | 8.9397 | 827.47 | 1.5875 |
| ν19 | 864.64 | 0.2246 | 858.99 | 0.138 |
| ν20 | 868.74 | 1.5064 | 867.8 | 1.2016 |
| ν21 | 889.83 | 1.0304 | 878.87 | 0.6124 |
| ν22 | 898.86 | 4.2587 | 894.99 | 2.4254 |
| ν23 | 911.81 | 0.0576 | 910.18 | 2.2615 |
| ν24 | 913.79 | 1.3419 | 915.62 | 0.2206 |
| ν25 | 926.56 | 0.9301 | 936.8 | 3.4974 |
| ν26 | 953.35 | 7.569 | 954.16 | 0.6611 |
| ν27 | 956.2 | 1.4766 | 971.33 | 11.1644 |
| ν28 | 987.35 | 2.9066 | 991.28 | 4.8185 |
| ν29 | 1006.42 | 4.7284 | 995.74 | 8.0401 |
| ν30 | 1032.25 | 2.7951 | 1004.28 | 7.3196 |
| ν31 | 1035.93 | 2.4614 | 1039.9 | 0.4124 |
| ν32 | 1041.62 | 1.4192 | 1048.14 | 3.5134 |
| ν33 | 1051.29 | 0.006 | 1050.55 | 2.079 |
| ν34 | 1079.33 | 0.6731 | 1062.7 | 0.2715 |
| ν35 | 1136.12 | 6.1294 | 1091.93 | 2.416 |
| ν36 | 1137.11 | 3.347 | 1118.88 | 3.3018 |
| ν37 | 1154.01 | 0.5803 | 1148.21 | 3.9525 |
| ν38 | 1174.46 | 6.7857 | 1178.95 | 7.1977 |
| ν39 | 1192.74 | 1.1719 | 1193.09 | 0.5238 |
| ν40 | 1196.21 | 1.2977 | 1201.14 | 0.6267 |
| ν41 | 1213.99 | 0.6269 | 1212.24 | 4.8875 |
| ν42 | 1225.96 | 4.2398 | 1230.02 | 3.2782 |
| ν43 | 1249.36 | 8.5277 | 1251.3 | 3.0854 |
| ν44 | 1261.03 | 2.0505 | 1260.76 | 0.5367 |
| ν45 | 1288.42 | 1.2536 | 1271.8 | 1.2113 |
| ν46 | 1291.83 | 1.2551 | 1298.9 | 1.9059 |
| ν47 | 1304.31 | 0.3851 | 1306.61 | 3.5262 |
| ν48 | 1312.48 | 0.2264 | 1314.11 | 0.6568 |
| ν49 | 1320.93 | 0.3974 | 1320.16 | 0.2144 |
| ν50 | 1325.16 | 1.3528 | 1326.91 | 1.7673 |
| ν51 | 1328.86 | 1.7959 | 1338.23 | 1.36 |
| ν52 | 1343.12 | 0.747 | 1344.08 | 0.456 |
| ν53 | 1349.14 | 0.5234 | 1360.65 | 1.1517 |
| ν54 | 1363.19 | 1.814 | 1371.09 | 0.2161 |
| ν55 | 1370.15 | 0.4695 | 1493.23 | 0.6478 |
| ν56 | 1482.32 | 6.0591 | 1493.93 | 1.1189 |
| ν57 | 1495.35 | 2.1346 | 1496.47 | 2.0157 |
| ν58 | 1496.83 | 2.726 | 1502.15 | 7.1454 |
| ν59 | 1507.49 | 3.9428 | 1512.43 | 7.269 |
| ν60 | 1521.1 | 9.8328 | 1524.61 | 6.2709 |
| ν61 | 3019.55 | 21.3664 | 3019.65 | 21.5207 |
| ν62 | 3025.86 | 28.2259 | 3026.81 | 28.3738 |
| ν63 | 3029.44 | 19.9982 | 3038.97 | 12.1392 |
| ν64 | 3030.67 | 26.5356 | 3041.02 | 5.8513 |
| ν65 | 3034.45 | 3.069 | 3045.17 | 29.4561 |
| ν66 | 3048.11 | 34.6066 | 3056.6 | 5.0664 |
| ν67 | 3062.45 | 12.6764 | 3059.38 | 67.8769 |
| ν68 | 3062.97 | 14.7917 | 3065.19 | 14.1679 |
| ν69 | 3071.6 | 43.053 | 3072.89 | 29.6595 |
| ν70 | 3075.27 | 42.8529 | 3077.22 | 25.7547 |
| ν71 | 3082.4 | 66.29 | 3077.87 | 54.9347 |
| ν72 | 3083.28 | 55.2831 | 3080.85 | 27.1755 |
| ν73 | 3087.05 | 43.0799 | 3089.7 | 46.8997 |
| ν74 | 3094.29 | 17.7348 | 3102.22 | 53.1647 |
| ν75 | 3106.81 | 24.8145 | 3115.32 | 26.9397 |
|  | **tsR3-OH** | | **tsR4-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -1301.13 | 599.9046 | -655.93 | 619.5207 |
| ν2 | 85.89 | 2.0128 | 79.03 | 1.7397 |
| ν3 | 88.77 | 2.2444 | 87.44 | 2.3239 |
| ν4 | 131.11 | 0.4323 | 146.12 | 0.5478 |
| ν5 | 174.21 | 0.569 | 172.36 | 1.1252 |
| ν6 | 263.5 | 0.282 | 268.07 | 0.584 |
| ν7 | 282.06 | 0.7367 | 307.71 | 2.3507 |
| ν8 | 315.04 | 0.0084 | 317.58 | 0.1673 |
| ν9 | 372 | 0.798 | 393.96 | 0.0327 |
| ν10 | 432.37 | 0.1411 | 479.17 | 22.4097 |
| ν11 | 535.37 | 0.087 | 532.7 | 4.2869 |
| ν12 | 553.85 | 3.2082 | 552.67 | 10.9825 |
| ν13 | 607.89 | 11.8973 | 568.08 | 138.4318 |
| ν14 | 665.43 | 1.4587 | 695.62 | 23.6959 |
| ν15 | 737.06 | 1.6311 | 741.94 | 3.3278 |
| ν16 | 752.01 | 1.574 | 767.67 | 46.6427 |
| ν17 | 789.15 | 2.0476 | 796.21 | 1.9947 |
| ν18 | 835.58 | 6.2237 | 832.73 | 0.5416 |
| ν19 | 854.29 | 0.5683 | 860.27 | 1.8152 |
| ν20 | 863.9 | 0.0815 | 868.53 | 3.7245 |
| ν21 | 885.23 | 0.2812 | 885.97 | 2.6278 |
| ν22 | 888.25 | 0.7461 | 889.93 | 0.6212 |
| ν23 | 911.11 | 0.5375 | 908.74 | 0.0651 |
| ν24 | 915.67 | 0.0063 | 913.49 | 1.237 |
| ν25 | 927.78 | 3.0971 | 924.57 | 9.8232 |
| ν26 | 947.56 | 5.7733 | 955.38 | 3.4549 |
| ν27 | 973.69 | 1.8093 | 960.19 | 1.1229 |
| ν28 | 987.44 | 2.1968 | 991.33 | 6.0706 |
| ν29 | 992.23 | 1.411 | 1010.22 | 1.3798 |
| ν30 | 1031.37 | 3.772 | 1046.18 | 0.9294 |
| ν31 | 1036.07 | 2.7023 | 1048.29 | 1.4758 |
| ν32 | 1039.33 | 0.1646 | 1052.78 | 1.9537 |
| ν33 | 1050.4 | 0.0408 | 1061.74 | 17.4861 |
| ν34 | 1074.32 | 0.6791 | 1076.51 | 2.0801 |
| ν35 | 1078.07 | 3.7279 | 1123.39 | 2.243 |
| ν36 | 1147.57 | 1.0357 | 1145.26 | 2.9123 |
| ν37 | 1163.56 | 17.3184 | 1152.18 | 4.6217 |
| ν38 | 1186.57 | 5.2459 | 1178.61 | 4.8426 |
| ν39 | 1193.51 | 0.4463 | 1190.77 | 1.6092 |
| ν40 | 1194.63 | 0.022 | 1198.35 | 5.8007 |
| ν41 | 1215.92 | 2.2093 | 1204.89 | 3.2327 |
| ν42 | 1232.14 | 2.2533 | 1224.46 | 0.2688 |
| ν43 | 1237.04 | 0.1604 | 1248.36 | 1.809 |
| ν44 | 1260.01 | 4.1101 | 1256.16 | 0.484 |
| ν45 | 1267.2 | 2.1424 | 1268.98 | 1.9735 |
| ν46 | 1287.15 | 0.0491 | 1291.31 | 1.123 |
| ν47 | 1303.31 | 0.0395 | 1307.92 | 0.2445 |
| ν48 | 1311.28 | 0.2544 | 1314.38 | 1.4222 |
| ν49 | 1318.15 | 0.16 | 1318.18 | 0.3237 |
| ν50 | 1327.63 | 0.3534 | 1331.21 | 1.2302 |
| ν51 | 1332.97 | 0.8895 | 1339.05 | 1.2264 |
| ν52 | 1342.95 | 0.5805 | 1345.22 | 1.2967 |
| ν53 | 1347.76 | 0.8957 | 1349.84 | 0.1563 |
| ν54 | 1361.98 | 0.1699 | 1358.61 | 0.4546 |
| ν55 | 1366.28 | 3.6244 | 1475.81 | 6.4612 |
| ν56 | 1469.2 | 0.0384 | 1493.72 | 1.3551 |
| ν57 | 1496.88 | 3.0291 | 1497.26 | 1.4702 |
| ν58 | 1497.29 | 4.7292 | 1501.8 | 6.0628 |
| ν59 | 1512.25 | 0.026 | 1509.71 | 9.4151 |
| ν60 | 1513.08 | 11.6834 | 1522 | 2.202 |
| ν61 | 3018.69 | 14.9679 | 3003.82 | 14.7823 |
| ν62 | 3023.46 | 28.0796 | 3022.95 | 14.3514 |
| ν63 | 3028.11 | 28.706 | 3034.12 | 21.4468 |
| ν64 | 3034.36 | 0.0053 | 3035.32 | 20.5331 |
| ν65 | 3046.29 | 29.4899 | 3042.26 | 28.2646 |
| ν66 | 3047.49 | 20.351 | 3047.98 | 29.1859 |
| ν67 | 3057.66 | 64.4634 | 3054.4 | 47.9652 |
| ν68 | 3072.86 | 37.2639 | 3072.78 | 23.5533 |
| ν69 | 3075 | 35.1829 | 3076.21 | 6.8386 |
| ν70 | 3077.3 | 10.6038 | 3077.66 | 55.7308 |
| ν71 | 3082 | 56.8219 | 3081.25 | 59.5346 |
| ν72 | 3091.96 | 62.5993 | 3084.35 | 38.2624 |
| ν73 | 3092.07 | 8.1117 | 3090.46 | 28.7693 |
| ν74 | 3102.08 | 37.0362 | 3093.52 | 33.7737 |
| ν75 | 3110.61 | 24.1379 | 3106.95 | 22.5549 |
|  | **tsR5-OH** | | **tsR6-OH** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -946.34 | 595.9346 | -922.56 | 745.9918 |
| ν2 | 64.73 | 1.3763 | 57.13 | 2.3371 |
| ν3 | 87.97 | 1.7397 | 75.08 | 2.0341 |
| ν4 | 142.37 | 0.6667 | 142.86 | 0.427 |
| ν5 | 195.92 | 0.8493 | 182.95 | 3.0993 |
| ν6 | 269.92 | 0.3515 | 263.26 | 0.1131 |
| ν7 | 310.69 | 2.2719 | 311.37 | 2.5877 |
| ν8 | 319.9 | 1.0452 | 320.25 | 0.4483 |
| ν9 | 396.96 | 0.3426 | 398.16 | 0.6244 |
| ν10 | 497.55 | 0.1428 | 490.21 | 0.0497 |
| ν11 | 529.65 | 3.6858 | 534.96 | 0.4385 |
| ν12 | 577.73 | 0.7433 | 579.94 | 10.924 |
| ν13 | 602.56 | 72.2332 | 639.19 | 96.7388 |
| ν14 | 697.35 | 2.973 | 672.68 | 0.9517 |
| ν15 | 738.3 | 0.7882 | 735.54 | 0.3537 |
| ν16 | 748.37 | 0.3382 | 758.78 | 5.7572 |
| ν17 | 792.12 | 3.3737 | 791.39 | 3.9104 |
| ν18 | 828.17 | 0.9957 | 828.64 | 1.5033 |
| ν19 | 857.73 | 2.7682 | 859.18 | 0.5428 |
| ν20 | 864.43 | 1.968 | 864.83 | 9.2874 |
| ν21 | 886.93 | 0.868 | 887.7 | 1.1158 |
| ν22 | 893.01 | 0.7778 | 887.92 | 0.1672 |
| ν23 | 910.35 | 1.1396 | 914.47 | 1.2901 |
| ν24 | 921.21 | 1.8638 | 915.25 | 0.5261 |
| ν25 | 925.13 | 0.9294 | 924.07 | 2.2371 |
| ν26 | 956.22 | 1.1111 | 954.56 | 0.9523 |
| ν27 | 960.94 | 0.0923 | 961.39 | 0.0034 |
| ν28 | 991.27 | 1.4005 | 992.87 | 2.7903 |
| ν29 | 997.89 | 2.4938 | 996.83 | 4.1753 |
| ν30 | 1034.85 | 0.3321 | 1037.81 | 2.6596 |
| ν31 | 1047.26 | 0.1999 | 1048.44 | 0.322 |
| ν32 | 1049.53 | 0.2236 | 1050.11 | 0.0393 |
| ν33 | 1053.55 | 0.0471 | 1062.01 | 0.8249 |
| ν34 | 1074.97 | 5.2227 | 1065.79 | 2.0044 |
| ν35 | 1112.13 | 8.8797 | 1133.9 | 0.254 |
| ν36 | 1140.3 | 0.8144 | 1141.18 | 2.0317 |
| ν37 | 1154.74 | 6.7027 | 1163.84 | 2.8746 |
| ν38 | 1167.81 | 1.4875 | 1169.41 | 3.2939 |
| ν39 | 1197.87 | 4.2131 | 1193.72 | 27.1512 |
| ν40 | 1204.49 | 2.1962 | 1200.93 | 0.2146 |
| ν41 | 1213.34 | 0.4806 | 1214.24 | 0.7013 |
| ν42 | 1225.02 | 2.6486 | 1233.29 | 2.0042 |
| ν43 | 1250.77 | 2.487 | 1239.77 | 0 |
| ν44 | 1276.39 | 1.8655 | 1258.38 | 0.0027 |
| ν45 | 1287.83 | 10.5341 | 1278.79 | 3.1371 |
| ν46 | 1293.49 | 0.728 | 1292.69 | 1.0688 |
| ν47 | 1301.58 | 3.8055 | 1306.67 | 0.0615 |
| ν48 | 1312.25 | 1.2006 | 1308 | 0.0007 |
| ν49 | 1316.34 | 0.5527 | 1312.59 | 2.3296 |
| ν50 | 1322.99 | 0.7779 | 1319.78 | 0.1982 |
| ν51 | 1331.88 | 0.9414 | 1326.37 | 0.4812 |
| ν52 | 1337.04 | 2.4507 | 1337.41 | 1.3539 |
| ν53 | 1348 | 4.9518 | 1353.01 | 3.2163 |
| ν54 | 1355.57 | 0.5492 | 1368.36 | 0.6661 |
| ν55 | 1368.35 | 0.4025 | 1371.22 | 0.1674 |
| ν56 | 1476.96 | 5.9225 | 1472.3 | 7.4279 |
| ν57 | 1495.71 | 1.2403 | 1482.17 | 2.0569 |
| ν58 | 1497.4 | 2.7705 | 1495.89 | 1.0462 |
| ν59 | 1508.23 | 10.8641 | 1505.5 | 11.3301 |
| ν60 | 1522.13 | 3.9041 | 1523.62 | 4.0251 |
| ν61 | 2988.67 | 18.0315 | 2988.62 | 7.3786 |
| ν62 | 3008.85 | 13.668 | 2992.57 | 15.2631 |
| ν63 | 3037.29 | 18.5197 | 3037.65 | 21.4573 |
| ν64 | 3039 | 33.0755 | 3046.02 | 44.9002 |
| ν65 | 3042.01 | 7.8687 | 3048.1 | 42.3535 |
| ν66 | 3043.91 | 42.5605 | 3049.96 | 0.4423 |
| ν67 | 3048.5 | 54.7978 | 3058.76 | 14.7804 |
| ν68 | 3065.7 | 2.2712 | 3066.62 | 0.5391 |
| ν69 | 3073.51 | 17.1549 | 3069.31 | 39.381 |
| ν70 | 3079.45 | 51.2641 | 3073.86 | 89.2775 |
| ν71 | 3081.36 | 40.5813 | 3073.86 | 28.7372 |
| ν72 | 3084.75 | 42.5557 | 3081.69 | 6.1464 |
| ν73 | 3087.01 | 13.9289 | 3086.31 | 39.2842 |
| ν74 | 3088.03 | 79.5672 | 3089.69 | 73.8952 |
| ν75 | 3094.96 | 28.825 | 3090.89 | 34.5264 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW R1-O2H** | | **vdW R2-O2H** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 24.68 | 1.5639 | 24.01 | 1.3122 |
| ν2 | 32.33 | 1.3439 | 53.57 | 0.829 |
| ν3 | 57.27 | 0.0517 | 57.03 | 0.8597 |
| ν4 | 93.05 | 0.3479 | 99.18 | 0.9423 |
| ν5 | 130.73 | 4.3947 | 138.32 | 0.0056 |
| ν6 | 164.63 | 1.9729 | 179.49 | 0.9171 |
| ν7 | 186.66 | 2.1611 | 200.47 | 11.0995 |
| ν8 | 301 | 0.4818 | 261.96 | 0.4994 |
| ν9 | 316.55 | 0.1732 | 316.31 | 0.233 |
| ν10 | 353.05 | 0.5826 | 330.45 | 0.1032 |
| ν11 | 407.51 | 0.1103 | 397.38 | 0.0254 |
| ν12 | 490.84 | 1.2629 | 484.96 | 0.4098 |
| ν13 | 539.48 | 0.266 | 515.96 | 2.331 |
| ν14 | 549.57 | 1.0159 | 544.14 | 0.6776 |
| ν15 | 607.84 | 19.9738 | 622.3 | 75.2357 |
| ν16 | 627.88 | 53.744 | 652.71 | 0.6565 |
| ν17 | 674.58 | 0.4392 | 724.63 | 0.217 |
| ν18 | 746.62 | 0.38 | 758.23 | 0.184 |
| ν19 | 765.84 | 0.2468 | 800.71 | 0.7757 |
| ν20 | 791.83 | 1.9541 | 829.64 | 0.7453 |
| ν21 | 856.22 | 0.9074 | 855.68 | 1.9692 |
| ν22 | 863.48 | 0.0347 | 875.32 | 0.4134 |
| ν23 | 884.46 | 0.3421 | 891.23 | 0.1546 |
| ν24 | 897.56 | 0.3446 | 912.05 | 0.5392 |
| ν25 | 910.06 | 0.1087 | 923.8 | 0.253 |
| ν26 | 913.09 | 0.8231 | 938.38 | 1.3756 |
| ν27 | 930.07 | 0.1834 | 955.6 | 1.4649 |
| ν28 | 950.45 | 1.8406 | 967.46 | 0.8419 |
| ν29 | 958.01 | 3.6533 | 990.06 | 0.2337 |
| ν30 | 982.42 | 1.3846 | 1013.23 | 0.3991 |
| ν31 | 990.25 | 1.7006 | 1018.3 | 1.4902 |
| ν32 | 998.53 | 0.9648 | 1052.48 | 0.0654 |
| ν33 | 1039.53 | 0.371 | 1057.69 | 0.0664 |
| ν34 | 1049.15 | 0.1252 | 1068.18 | 0.5291 |
| ν35 | 1054.5 | 0.6244 | 1097.16 | 0.4192 |
| ν36 | 1067.31 | 1.1524 | 1119.43 | 0.3362 |
| ν37 | 1118.26 | 0.2743 | 1147.61 | 1.4395 |
| ν38 | 1141.06 | 0.2546 | 1167.94 | 1.9407 |
| ν39 | 1162.18 | 1.2372 | 1196.41 | 0.0724 |
| ν40 | 1178.33 | 15.0418 | 1198.6 | 1.4412 |
| ν41 | 1187.13 | 0.6067 | 1208.63 | 3.829 |
| ν42 | 1195.28 | 0.3186 | 1219.75 | 2.1416 |
| ν43 | 1209.01 | 0.3813 | 1233.04 | 3.0346 |
| ν44 | 1229.46 | 0.4533 | 1256.84 | 0.1331 |
| ν45 | 1254.95 | 1.3583 | 1262.08 | 23.56 |
| ν46 | 1279.95 | 1.5245 | 1267.51 | 36.5368 |
| ν47 | 1286.32 | 0.6502 | 1279.57 | 2.058 |
| ν48 | 1304.15 | 0.4802 | 1292.52 | 1.1092 |
| ν49 | 1309.09 | 0.1748 | 1308.86 | 0.3041 |
| ν50 | 1320.81 | 0.33 | 1312.03 | 1.0826 |
| ν51 | 1324.8 | 0.3647 | 1315.52 | 0.729 |
| ν52 | 1335.15 | 1.0473 | 1327.84 | 0.4506 |
| ν53 | 1344.71 | 0.746 | 1344.48 | 0.0141 |
| ν54 | 1348.12 | 0.7632 | 1353.83 | 0.4681 |
| ν55 | 1364.63 | 0.4836 | 1372.29 | 0.8754 |
| ν56 | 1370.76 | 0.4613 | 1470.95 | 1.2164 |
| ν57 | 1470.79 | 6.1704 | 1472.78 | 0.227 |
| ν58 | 1495.14 | 1.7565 | 1478.47 | 2.1214 |
| ν59 | 1497.25 | 3.0625 | 1483.76 | 10.4259 |
| ν60 | 1502.55 | 10.2434 | 1496.92 | 6.7809 |
| ν61 | 1507.33 | 9.6349 | 1506.17 | 6.9355 |
| ν62 | 1520.76 | 8.3029 | 1521.02 | 18.3033 |
| ν63 | 2951.94 | 304.6055 | 3071.88 | 406.3918 |
| ν64 | 2993.29 | 35.409 | 3080.52 | 24.5839 |
| ν65 | 3020.25 | 13.0456 | 3083.11 | 28.8543 |
| ν66 | 3020.64 | 19.4068 | 3087.07 | 25.162 |
| ν67 | 3024.91 | 29.7649 | 3092.82 | 20.2697 |
| ν68 | 3029.93 | 27.1104 | 3094.96 | 18.0435 |
| ν69 | 3040.49 | 8.862 | 3106.52 | 38.5109 |
| ν70 | 3055.2 | 42.5611 | 3112.72 | 20.2411 |
| ν71 | 3057.53 | 20.7549 | 3128.82 | 32.9195 |
| ν72 | 3072.99 | 34.3008 | 3131.84 | 6.6612 |
| ν73 | 3076.45 | 43.2845 | 3147.89 | 23.8241 |
| ν74 | 3084.23 | 81.8866 | 3154.98 | 11.1563 |
| ν75 | 3086.67 | 42.1779 | 3155.47 | 27.5404 |
| ν76 | 3098.68 | 18.9452 | 3169.85 | 19.6185 |
| ν77 | 3099.77 | 29.6955 | 3177.02 | 25.7186 |
| ν78 | 3150.07 | 7.9329 | 3186.6 | 18.3915 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW R3-O2H** | | **vdW R4-O2H** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 32.31 | 1.2021 | 34.06 | 1.1821 |
| ν2 | 41.95 | 1.611 | 60.23 | 0.4826 |
| ν3 | 61.8 | 0.0183 | 68.18 | 0.7221 |
| ν4 | 74.33 | 0.2362 | 112.76 | 0.4758 |
| ν5 | 123.86 | 0.034 | 124.5 | 0.2239 |
| ν6 | 147.75 | 3.8694 | 179.81 | 0.2528 |
| ν7 | 199.68 | 1.9581 | 208.07 | 9.91 |
| ν8 | 256.19 | 0.2385 | 250.42 | 0.5524 |
| ν9 | 310.98 | 0.0396 | 305.02 | 1.2092 |
| ν10 | 314.8 | 0.0062 | 320.52 | 0.1278 |
| ν11 | 402.15 | 0.1989 | 389.11 | 0.0359 |
| ν12 | 532.38 | 0.1071 | 479.04 | 0.8115 |
| ν13 | 536.13 | 3.3212 | 533.7 | 0.5474 |
| ν14 | 551.36 | 2.2442 | 545.67 | 0.8747 |
| ν15 | 666.13 | 14.1625 | 633.46 | 3.8686 |
| ν16 | 691.41 | 30.5727 | 663.36 | 72.4388 |
| ν17 | 727.4 | 0.0473 | 726.92 | 0.6222 |
| ν18 | 757.82 | 0.597 | 751.21 | 1.1399 |
| ν19 | 787.31 | 0.1788 | 807.09 | 1.6468 |
| ν20 | 807.19 | 3.3968 | 829.83 | 2.4436 |
| ν21 | 840.54 | 2.348 | 862.54 | 0.2414 |
| ν22 | 851.93 | 0.0467 | 892.31 | 0.3084 |
| ν23 | 868.27 | 0.0652 | 894.82 | 1.78 |
| ν24 | 874.63 | 1.4551 | 912.66 | 0.6329 |
| ν25 | 912.25 | 0.0027 | 916.9 | 0.1949 |
| ν26 | 916.05 | 1.78 | 931.75 | 0.0157 |
| ν27 | 921.6 | 0.0187 | 944.26 | 0.9742 |
| ν28 | 942.86 | 0.1425 | 969.61 | 2.9124 |
| ν29 | 946.59 | 0.3523 | 976.09 | 0.8631 |
| ν30 | 990.82 | 1.7113 | 1015.06 | 0.5472 |
| ν31 | 992.97 | 1.7709 | 1024.1 | 2.2832 |
| ν32 | 1002.24 | 0.2645 | 1047.8 | 0.4499 |
| ν33 | 1040.77 | 0.1772 | 1061.61 | 0.2833 |
| ν34 | 1052.26 | 0.0001 | 1067.04 | 0.1104 |
| ν35 | 1057.62 | 0.1849 | 1102.54 | 1.4185 |
| ν36 | 1071.59 | 0.7993 | 1131.52 | 0.0405 |
| ν37 | 1151.43 | 0.535 | 1136.84 | 0.0774 |
| ν38 | 1159.41 | 12.0202 | 1162.3 | 0.3228 |
| ν39 | 1179 | 14.585 | 1165.8 | 1.4778 |
| ν40 | 1192.83 | 2.2258 | 1195.98 | 2.5647 |
| ν41 | 1193.87 | 0.1747 | 1217.44 | 0.2749 |
| ν42 | 1204.02 | 0.8886 | 1229.4 | 4.6784 |
| ν43 | 1205.31 | 0.6793 | 1237.26 | 0.8397 |
| ν44 | 1235.35 | 1.8726 | 1247.51 | 0.3911 |
| ν45 | 1246.92 | 0.0005 | 1260.15 | 12.1313 |
| ν46 | 1261.05 | 1.0162 | 1265.25 | 46.4701 |
| ν47 | 1282.39 | 0.005 | 1271.05 | 0.2201 |
| ν48 | 1304.51 | 0.003 | 1298.97 | 0.513 |
| ν49 | 1311.96 | 0.3051 | 1305.23 | 0.1953 |
| ν50 | 1317.51 | 0.0001 | 1315.15 | 1.3696 |
| ν51 | 1327.7 | 0.029 | 1323.15 | 1.3132 |
| ν52 | 1332.76 | 0.7873 | 1338.62 | 0.5028 |
| ν53 | 1346.48 | 0.7266 | 1341.03 | 0.0272 |
| ν54 | 1350.04 | 0.0272 | 1350.44 | 0.4724 |
| ν55 | 1364.49 | 0.6901 | 1368.67 | 0.6883 |
| ν56 | 1369.68 | 0.3149 | 1454.45 | 7.0352 |
| ν57 | 1492.96 | 1.5202 | 1472.05 | 1.0282 |
| ν58 | 1493.35 | 3.3813 | 1477.47 | 1.741 |
| ν59 | 1497.78 | 2.8542 | 1482.72 | 8.3521 |
| ν60 | 1503.21 | 14.5985 | 1492.6 | 6.9192 |
| ν61 | 1509.46 | 4.5426 | 1506.37 | 4.7108 |
| ν62 | 1519.96 | 6.0171 | 1525.89 | 8.2544 |
| ν63 | 2626.18 | 88.7933 | 3037.75 | 36.1291 |
| ν64 | 3018.71 | 15.6357 | 3069.86 | 407.6858 |
| ν65 | 3025.1 | 24.97 | 3078.88 | 19.4352 |
| ν66 | 3029.89 | 28.6808 | 3083.13 | 2.9793 |
| ν67 | 3037.61 | 4.3652 | 3088.61 | 23.5368 |
| ν68 | 3041.36 | 24.866 | 3090.15 | 16.2005 |
| ν69 | 3048.77 | 14.6564 | 3094.76 | 16.4375 |
| ν70 | 3053.32 | 76.5299 | 3105.67 | 44.6255 |
| ν71 | 3073.76 | 7.9575 | 3116.48 | 27.5166 |
| ν72 | 3074.96 | 38.4207 | 3138.03 | 38.2969 |
| ν73 | 3075.6 | 31.2517 | 3148.81 | 19.9863 |
| ν74 | 3082.98 | 65.9086 | 3153.27 | 33.2007 |
| ν75 | 3093.92 | 47.8054 | 3157.67 | 1.4761 |
| ν76 | 3097.28 | 55.5116 | 3157.88 | 7.0162 |
| ν77 | 3097.98 | 9.341 | 3162.8 | 34.743 |
| ν78 | 3117.4 | 12.9118 | 3175.07 | 26.5958 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **vdW R5-O2H** | | **vdW R6-O2H** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | 18.45 | 1.524 | 19.36 | 1.3998 |
| ν2 | 36.34 | 1.2313 | 39.75 | 0.4617 |
| ν3 | 51.55 | 0.1552 | 52.97 | 1.0484 |
| ν4 | 90.82 | 0.2422 | 94.07 | 0.3113 |
| ν5 | 120.14 | 2.0982 | 126.86 | 0.3467 |
| ν6 | 144.51 | 0.3787 | 186.78 | 0.8231 |
| ν7 | 195.39 | 4.9313 | 201.96 | 8.7813 |
| ν8 | 269.86 | 0.2479 | 260.94 | 0.0168 |
| ν9 | 308.59 | 0.3787 | 281.01 | 1.0672 |
| ν10 | 333.41 | 1.2126 | 325.52 | 0.0796 |
| ν11 | 395.14 | 0.2343 | 395.98 | 0.5889 |
| ν12 | 491.83 | 0.4441 | 490.39 | 0.9203 |
| ν13 | 534.78 | 0.3398 | 533.32 | 0.4724 |
| ν14 | 581.91 | 11.2958 | 547.95 | 14.2294 |
| ν15 | 613.15 | 60.049 | 687.6 | 1.5465 |
| ν16 | 658.51 | 8.5592 | 692.59 | 40.7838 |
| ν17 | 736.94 | 0.3744 | 712.55 | 20.0851 |
| ν18 | 746.55 | 1.2586 | 732.12 | 0.4649 |
| ν19 | 781.84 | 4.004 | 778.3 | 0.938 |
| ν20 | 800.37 | 0.69 | 798.29 | 0.6912 |
| ν21 | 829.94 | 0.3486 | 828.37 | 1.0606 |
| ν22 | 850.08 | 0.5871 | 845.7 | 0.301 |
| ν23 | 870.39 | 1.5243 | 886.57 | 1.0281 |
| ν24 | 887.26 | 0.603 | 888.17 | 0.4948 |
| ν25 | 903.17 | 0.366 | 913.7 | 0.7071 |
| ν26 | 920.98 | 0.3723 | 923.75 | 1.0176 |
| ν27 | 924.63 | 1.2577 | 924.23 | 1.8734 |
| ν28 | 947.54 | 1.5656 | 948.65 | 0.5762 |
| ν29 | 961.36 | 0.2855 | 962.26 | 0.026 |
| ν30 | 981.28 | 1.1212 | 966.83 | 1.8278 |
| ν31 | 998.39 | 0.6324 | 1004.55 | 2.7674 |
| ν32 | 1017.42 | 0.9503 | 1024.47 | 0.5262 |
| ν33 | 1046.14 | 0.1196 | 1044.67 | 0.8787 |
| ν34 | 1049.67 | 0.1287 | 1051.82 | 0.8008 |
| ν35 | 1059.67 | 0.697 | 1058.67 | 0.4567 |
| ν36 | 1071.59 | 2.0018 | 1074.22 | 0.003 |
| ν37 | 1123.81 | 0.5861 | 1130.19 | 0.8499 |
| ν38 | 1143.55 | 0.1805 | 1145.54 | 0.101 |
| ν39 | 1161.82 | 0.7129 | 1153.01 | 0.4992 |
| ν40 | 1176.09 | 13.5192 | 1175.83 | 15.8454 |
| ν41 | 1186.53 | 2.2944 | 1192.01 | 3.7222 |
| ν42 | 1205.33 | 3.5316 | 1198.53 | 0.0185 |
| ν43 | 1218.65 | 0.3903 | 1213.09 | 1.2984 |
| ν44 | 1227.7 | 0.3719 | 1233.81 | 2.0236 |
| ν45 | 1248.21 | 0.2519 | 1249.71 | 0.4037 |
| ν46 | 1277.69 | 1.3171 | 1262.84 | 0.7614 |
| ν47 | 1288.05 | 1.3784 | 1292.65 | 1.0791 |
| ν48 | 1294.92 | 0.7951 | 1307.22 | 0.0509 |
| ν49 | 1301.66 | 0.4167 | 1308.93 | 0.6173 |
| ν50 | 1314.78 | 0.2572 | 1311.3 | 0.3579 |
| ν51 | 1319.8 | 1.6941 | 1321.91 | 1.201 |
| ν52 | 1324.06 | 0.4398 | 1327.06 | 1.6529 |
| ν53 | 1335.84 | 1.8757 | 1346.17 | 0.3133 |
| ν54 | 1349.17 | 1.6194 | 1354.71 | 4.0234 |
| ν55 | 1362.48 | 0.6573 | 1365.62 | 0.1477 |
| ν56 | 1368.91 | 1.0759 | 1370.71 | 0.8852 |
| ν57 | 1469.02 | 4.0518 | 1458.81 | 19.8817 |
| ν58 | 1492.55 | 14.3168 | 1468.63 | 4.2905 |
| ν59 | 1495.91 | 0.8417 | 1496.31 | 1.0858 |
| ν60 | 1497.7 | 3.8445 | 1504.17 | 9.2433 |
| ν61 | 1509.92 | 11.3912 | 1507.2 | 9.2372 |
| ν62 | 1522.78 | 1.6135 | 1523.21 | 3.9234 |
| ν63 | 2935.27 | 29.6311 | 2785.53 | 199.0387 |
| ν64 | 2971.51 | 30.7998 | 2938.86 | 13.6759 |
| ν65 | 2999.53 | 247.1953 | 2941.98 | 20.9887 |
| ν66 | 3034.28 | 26.2647 | 3024.6 | 16.6952 |
| ν67 | 3039.18 | 25.6884 | 3033.3 | 5.8841 |
| ν68 | 3046.41 | 12.3807 | 3038.25 | 19.7717 |
| ν69 | 3046.99 | 9.1826 | 3044.82 | 37.4833 |
| ν70 | 3049.21 | 107.1955 | 3048.46 | 48.8684 |
| ν71 | 3051.8 | 12.6307 | 3054.24 | 13.8542 |
| ν72 | 3067.75 | 3.5407 | 3067.56 | 14.5735 |
| ν73 | 3079.77 | 51.9366 | 3069 | 28.6668 |
| ν74 | 3084.27 | 43.1111 | 3074.65 | 75.1828 |
| ν75 | 3088.44 | 35.7434 | 3081.99 | 2.9094 |
| ν76 | 3091.98 | 47.0152 | 3084.57 | 33.5859 |
| ν77 | 3092.43 | 44.1936 | 3089.95 | 79.4418 |
| ν78 | 3132.18 | 7.9185 | 3140.56 | 28.4242 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **tsR1-O2H** | |  | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -507.33 | 87.3089 |  |  |
| ν2 | 25.69 | 1.1685 |  |  |
| ν3 | 41.71 | 1.2673 |  |  |
| ν4 | 74.86 | 0.2723 |  |  |
| ν5 | 138.03 | 1.246 |  |  |
| ν6 | 164.3 | 0.4884 |  |  |
| ν7 | 176.1 | 0.0733 |  |  |
| ν8 | 299.18 | 0.7187 |  |  |
| ν9 | 315.47 | 0.1615 |  |  |
| ν10 | 328.88 | 3.536 |  |  |
| ν11 | 400.28 | 2.7662 |  |  |
| ν12 | 489.81 | 1.3566 |  |  |
| ν13 | 533.85 | 0.4938 |  |  |
| ν14 | 555.8 | 0.4071 |  |  |
| ν15 | 623.93 | 8.2114 |  |  |
| ν16 | 675.09 | 1.0007 |  |  |
| ν17 | 744.11 | 1.557 |  |  |
| ν18 | 760.35 | 6.8655 |  |  |
| ν19 | 792.37 | 1.4527 |  |  |
| ν20 | 844.45 | 8.0192 |  |  |
| ν21 | 861.85 | 1.9815 |  |  |
| ν22 | 871.58 | 22.3855 |  |  |
| ν23 | 875.9 | 7.5775 |  |  |
| ν24 | 895.48 | 5.334 |  |  |
| ν25 | 909.97 | 1.5336 |  |  |
| ν26 | 911.25 | 0.47 |  |  |
| ν27 | 927.3 | 1.962 |  |  |
| ν28 | 952.01 | 4.9997 |  |  |
| ν29 | 957.91 | 5.0076 |  |  |
| ν30 | 978.78 | 3.8228 |  |  |
| ν31 | 991.49 | 1.7425 |  |  |
| ν32 | 995.66 | 3.7744 |  |  |
| ν33 | 1041.12 | 0.7253 |  |  |
| ν34 | 1050.45 | 1.2523 |  |  |
| ν35 | 1058.9 | 1.0805 |  |  |
| ν36 | 1063.29 | 7.3434 |  |  |
| ν37 | 1105.33 | 14.6627 |  |  |
| ν38 | 1135.1 | 3.8423 |  |  |
| ν39 | 1156.54 | 8.1609 |  |  |
| ν40 | 1173.32 | 17.618 |  |  |
| ν41 | 1189.68 | 0.3909 |  |  |
| ν42 | 1195.71 | 0.3819 |  |  |
| ν43 | 1210.53 | 1.0375 |  |  |
| ν44 | 1227.82 | 0.3158 |  |  |
| ν45 | 1256.21 | 0.9646 |  |  |
| ν46 | 1279.23 | 1.0453 |  |  |
| ν47 | 1290.32 | 0.4718 |  |  |
| ν48 | 1305.17 | 0.4328 |  |  |
| ν49 | 1310.3 | 0.3509 |  |  |
| ν50 | 1320.58 | 0.2665 |  |  |
| ν51 | 1323.84 | 0.1224 |  |  |
| ν52 | 1330.83 | 1.6671 |  |  |
| ν53 | 1344.55 | 0.6303 |  |  |
| ν54 | 1349.15 | 1.2455 |  |  |
| ν55 | 1366.12 | 0.307 |  |  |
| ν56 | 1373.41 | 0.5273 |  |  |
| ν57 | 1469.78 | 3.2453 |  |  |
| ν58 | 1473.74 | 6.6858 |  |  |
| ν59 | 1495.2 | 1.815 |  |  |
| ν60 | 1497.07 | 2.9768 |  |  |
| ν61 | 1506.79 | 5.4828 |  |  |
| ν62 | 1520.53 | 8.3178 |  |  |
| ν63 | 1674.77 | 11.6324 |  |  |
| ν64 | 3007.99 | 26.5795 |  |  |
| ν65 | 3020.31 | 12.8411 |  |  |
| ν66 | 3024.51 | 27.7991 |  |  |
| ν67 | 3029.35 | 26.9983 |  |  |
| ν68 | 3033.56 | 7.9443 |  |  |
| ν69 | 3042.94 | 16.028 |  |  |
| ν70 | 3054.55 | 32.5081 |  |  |
| ν71 | 3062.5 | 20.4839 |  |  |
| ν72 | 3073.34 | 33.6736 |  |  |
| ν73 | 3076.72 | 42.6568 |  |  |
| ν74 | 3084.78 | 89.2472 |  |  |
| ν75 | 3085.77 | 31.5698 |  |  |
| ν76 | 3097.07 | 11.6038 |  |  |
| ν77 | 3098.87 | 36.0451 |  |  |
| ν78 | 3117.51 | 19.1249 |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **tsR3-O2H** | | **tsR4-O2H** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -114.09 | 3.999 | -1429.39 | 350.373 |
| ν2 | 33.74 | 1.1147 | 36.26 | 1.5682 |
| ν3 | 51.04 | 1.3224 | 78.18 | 0.7212 |
| ν4 | 68.36 | 0.0567 | 96.27 | 0.9742 |
| ν5 | 125.15 | 0.0339 | 142.44 | 0.3441 |
| ν6 | 149.41 | 2.0056 | 161.25 | 0.6585 |
| ν7 | 197.94 | 0.8471 | 227.96 | 1.4425 |
| ν8 | 256.68 | 0.242 | 270.96 | 0.267 |
| ν9 | 311.91 | 0.0665 | 305.55 | 0.0754 |
| ν10 | 314.31 | 0.0049 | 328.99 | 0.0271 |
| ν11 | 399.23 | 1.2796 | 389.81 | 0.7861 |
| ν12 | 532.28 | 0.2078 | 421.1 | 3.1698 |
| ν13 | 548.11 | 0.4209 | 506.41 | 1.275 |
| ν14 | 556.9 | 7.5824 | 533.55 | 0.2969 |
| ν15 | 670.95 | 1.3091 | 546.07 | 1.3554 |
| ν16 | 722.8 | 7.4411 | 691.92 | 2.3131 |
| ν17 | 754.07 | 0.3711 | 750.7 | 0.9209 |
| ν18 | 767.5 | 29.9022 | 784.13 | 2.3903 |
| ν19 | 779.23 | 1.3504 | 813.64 | 1.198 |
| ν20 | 811.64 | 0.5118 | 848.6 | 4.1051 |
| ν21 | 834.69 | 4.5461 | 874.72 | 2.0878 |
| ν22 | 852.79 | 0.0008 | 893.56 | 2.3892 |
| ν23 | 868.77 | 0.1146 | 909.47 | 1.4507 |
| ν24 | 874.74 | 0.471 | 915.37 | 0.3906 |
| ν25 | 912.78 | 0.0022 | 930.05 | 1.181 |
| ν26 | 915.54 | 1.3656 | 934.52 | 0.5078 |
| ν27 | 922.87 | 0.1733 | 947.83 | 2.2671 |
| ν28 | 937.52 | 1.171 | 969.21 | 3.1675 |
| ν29 | 946.42 | 0.3309 | 977.09 | 1.712 |
| ν30 | 990.77 | 2.6082 | 1000.86 | 23.1104 |
| ν31 | 993.6 | 1.7226 | 1022.3 | 7.0845 |
| ν32 | 1003.78 | 0.4361 | 1031.23 | 3.536 |
| ν33 | 1041.17 | 0.2572 | 1051.62 | 2.0948 |
| ν34 | 1052.2 | 0.0016 | 1065.6 | 0.6757 |
| ν35 | 1058.57 | 0.1974 | 1070.76 | 0.1631 |
| ν36 | 1071.35 | 1.7521 | 1100.12 | 1.102 |
| ν37 | 1149.6 | 33.3973 | 1134.88 | 0.9068 |
| ν38 | 1151.2 | 0.4968 | 1144.52 | 2.208 |
| ν39 | 1179.08 | 11.7515 | 1160.9 | 1.2194 |
| ν40 | 1193.79 | 0.1579 | 1194.38 | 4.9277 |
| ν41 | 1195.81 | 4.2723 | 1197.31 | 2.5264 |
| ν42 | 1204.11 | 0.6797 | 1216.91 | 1.5411 |
| ν43 | 1205.51 | 0.6213 | 1232.74 | 2.3179 |
| ν44 | 1234.94 | 2.1293 | 1236.2 | 0.0935 |
| ν45 | 1246.76 | 0.0001 | 1250.23 | 0.5285 |
| ν46 | 1261.48 | 0.8613 | 1264.9 | 0.3631 |
| ν47 | 1283 | 0.005 | 1271.78 | 0.9724 |
| ν48 | 1304.76 | 0.0038 | 1300.55 | 0.2431 |
| ν49 | 1312.32 | 0.422 | 1305.81 | 0.9032 |
| ν50 | 1317.39 | 0.0017 | 1315.08 | 1.6782 |
| ν51 | 1327.89 | 0.0437 | 1323.92 | 1.3681 |
| ν52 | 1332.76 | 0.9229 | 1337.68 | 0.249 |
| ν53 | 1346.43 | 0.6953 | 1341.97 | 0.0574 |
| ν54 | 1350.35 | 0.0141 | 1349.68 | 1.0468 |
| ν55 | 1364.37 | 0.5752 | 1362.79 | 0.4603 |
| ν56 | 1369.75 | 0.3088 | 1417.39 | 19.2351 |
| ν57 | 1492.9 | 1.5094 | 1455.83 | 5.5837 |
| ν58 | 1494.68 | 2.0905 | 1472.41 | 1.2312 |
| ν59 | 1498.04 | 2.9327 | 1477.59 | 2.3304 |
| ν60 | 1505.09 | 11.7862 | 1483.52 | 8.2622 |
| ν61 | 1509.49 | 5.1595 | 1493.28 | 6.5137 |
| ν62 | 1522.64 | 5.8166 | 1507.92 | 3.4634 |
| ν63 | 2182.23 | 7.4846 | 1542.04 | 13.4645 |
| ν64 | 3019.37 | 19.5244 | 3046.74 | 16.6449 |
| ν65 | 3027.85 | 26.286 | 3078.08 | 10.0615 |
| ν66 | 3032 | 21.9442 | 3082.32 | 5.3467 |
| ν67 | 3037.46 | 4.6228 | 3089.24 | 21.936 |
| ν68 | 3041.36 | 24.9056 | 3090.79 | 28.1157 |
| ν69 | 3048.72 | 13.6604 | 3094.82 | 17.2205 |
| ν70 | 3053.19 | 79.6952 | 3106.59 | 38.6715 |
| ν71 | 3073.86 | 4.2216 | 3125.62 | 16.492 |
| ν72 | 3075.33 | 40.6523 | 3136.79 | 39.7446 |
| ν73 | 3075.75 | 31.606 | 3146.69 | 20.5253 |
| ν74 | 3083.6 | 64.7872 | 3153.3 | 32.0551 |
| ν75 | 3093.65 | 39.555 | 3157.65 | 3.3491 |
| ν76 | 3095.58 | 15.3675 | 3158.46 | 8.5779 |
| ν77 | 3097 | 55.4044 | 3162.79 | 30.7729 |
| ν78 | 3109.25 | 17.2621 | 3177.11 | 20.9041 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **tsR5-O2H** | | **tsR6-O2H** | |
| Normal modes | Frequency(cm-1) | IR Inten | Frequency(cm-1) | IR Inten |
| ν1 | -716.37 | 174.5419 | -419.76 | 30.6858 |
| ν2 | 11.53 | 1.1077 | 26.74 | 1.4338 |
| ν3 | 54.52 | 1.0525 | 50.59 | 0.4635 |
| ν4 | 70.97 | 0.4327 | 63.98 | 1.0036 |
| ν5 | 132.2 | 0.168 | 134.53 | 0.9436 |
| ν6 | 159.78 | 1.2114 | 136.92 | 0.0253 |
| ν7 | 175.38 | 0.0948 | 238.93 | 1.6433 |
| ν8 | 269.25 | 0.3882 | 264.39 | 0.0773 |
| ν9 | 291.78 | 1.3957 | 288.89 | 0.3795 |
| ν10 | 319.78 | 0.5222 | 331.14 | 0.1138 |
| ν11 | 395.77 | 0.1272 | 397.07 | 0.8335 |
| ν12 | 495.8 | 0.648 | 492.42 | 0.7711 |
| ν13 | 532.64 | 1.0127 | 534.6 | 0.1062 |
| ν14 | 600.15 | 1.3879 | 568.23 | 3.059 |
| ν15 | 644.25 | 11.0005 | 685.44 | 0.3926 |
| ν16 | 735.78 | 0.9598 | 702.02 | 5.8043 |
| ν17 | 745.99 | 0.1226 | 733.22 | 0.3734 |
| ν18 | 770.6 | 10.2864 | 781.08 | 0.276 |
| ν19 | 793.19 | 6.3382 | 795.96 | 6.1231 |
| ν20 | 827.96 | 1.8492 | 827.94 | 2.6429 |
| ν21 | 847.04 | 7.4273 | 848.93 | 0.2959 |
| ν22 | 860.38 | 4.4339 | 886.86 | 1.8852 |
| ν23 | 887.38 | 0.811 | 887.61 | 1.1277 |
| ν24 | 889.28 | 11.8902 | 894.37 | 26.7081 |
| ν25 | 908.74 | 18.3546 | 910.9 | 8.6293 |
| ν26 | 912.38 | 5.1111 | 922.67 | 3.4347 |
| ν27 | 923.88 | 0.8485 | 924.52 | 3.2344 |
| ν28 | 951.15 | 5.6343 | 929.28 | 19.7909 |
| ν29 | 961.14 | 0.6407 | 962.17 | 0.0795 |
| ν30 | 983.75 | 12.2083 | 963.48 | 9.9241 |
| ν31 | 987.64 | 2.0908 | 1003.02 | 2.832 |
| ν32 | 1011.17 | 6.8354 | 1016.13 | 9.9875 |
| ν33 | 1035.33 | 10.7554 | 1046.22 | 0.6794 |
| ν34 | 1049.25 | 3.0756 | 1051.99 | 0.6426 |
| ν35 | 1050.28 | 0.1808 | 1057.75 | 3.2557 |
| ν36 | 1058.69 | 2.0102 | 1075.56 | 0.0114 |
| ν37 | 1095.98 | 13.981 | 1108.46 | 37.4992 |
| ν38 | 1140.41 | 2.2916 | 1132.2 | 0.8842 |
| ν39 | 1157.86 | 6.6953 | 1146.84 | 0.05 |
| ν40 | 1163.42 | 0.7126 | 1167.1 | 10.3544 |
| ν41 | 1197.51 | 4.4788 | 1199.3 | 0.024 |
| ν42 | 1203.94 | 4.7689 | 1209.76 | 3.9474 |
| ν43 | 1219.07 | 0.2409 | 1214.41 | 1.9075 |
| ν44 | 1225.14 | 0.8788 | 1236.6 | 2.7532 |
| ν45 | 1249.51 | 0.5167 | 1247.17 | 0.69 |
| ν46 | 1276.46 | 1.5214 | 1259.83 | 0.5131 |
| ν47 | 1289.32 | 1.0117 | 1293.14 | 1.1107 |
| ν48 | 1294.97 | 1.6672 | 1307.63 | 0.0561 |
| ν49 | 1302.33 | 1.0462 | 1310.32 | 1.8178 |
| ν50 | 1315.76 | 0.4763 | 1311.29 | 0.3221 |
| ν51 | 1318.19 | 1.6682 | 1321.3 | 1.7202 |
| ν52 | 1324.53 | 0.5539 | 1326.16 | 1.3754 |
| ν53 | 1335.71 | 1.5413 | 1344.4 | 0.5109 |
| ν54 | 1348.22 | 3.2167 | 1354.18 | 4.9442 |
| ν55 | 1359.04 | 0.3854 | 1365.48 | 0.29 |
| ν56 | 1367.98 | 0.6056 | 1369.65 | 0.7588 |
| ν57 | 1422.88 | 1.6119 | 1458.37 | 17.9869 |
| ν58 | 1471.12 | 4.5909 | 1469.87 | 4.773 |
| ν59 | 1496.04 | 1.2596 | 1492.36 | 1.3606 |
| ν60 | 1498.76 | 2.0571 | 1496 | 1.2026 |
| ν61 | 1508.58 | 12.2207 | 1504.88 | 10.6079 |
| ν62 | 1523.48 | 4.0006 | 1523.67 | 4.1736 |
| ν63 | 1589.71 | 13.4338 | 1716.93 | 10.1756 |
| ν64 | 2951.66 | 21.4571 | 2949.84 | 11.4299 |
| ν65 | 2982.48 | 20.1287 | 2953.21 | 21.9928 |
| ν66 | 3037.35 | 7.6821 | 3032.47 | 14.3828 |
| ν67 | 3038.76 | 31.3387 | 3035.93 | 5.4257 |
| ν68 | 3045.07 | 13.6183 | 3038.34 | 18.5954 |
| ν69 | 3048.98 | 73.904 | 3045.66 | 38.5631 |
| ν70 | 3052.95 | 28.8134 | 3048.57 | 47.5375 |
| ν71 | 3054.13 | 15.7368 | 3054.61 | 14.4922 |
| ν72 | 3067.21 | 2.9892 | 3067.65 | 15.3314 |
| ν73 | 3079.93 | 48.0367 | 3068.67 | 25.0619 |
| ν74 | 3084.78 | 44.781 | 3074.77 | 75.8192 |
| ν75 | 3088.51 | 51.2097 | 3082.04 | 4.4966 |
| ν76 | 3092.82 | 36.9823 | 3085.5 | 32.7305 |
| ν77 | 3098.74 | 29.4799 | 3090.07 | 79.3461 |
| ν78 | 3105.54 | 15.2297 | 3123.43 | 30.057 |