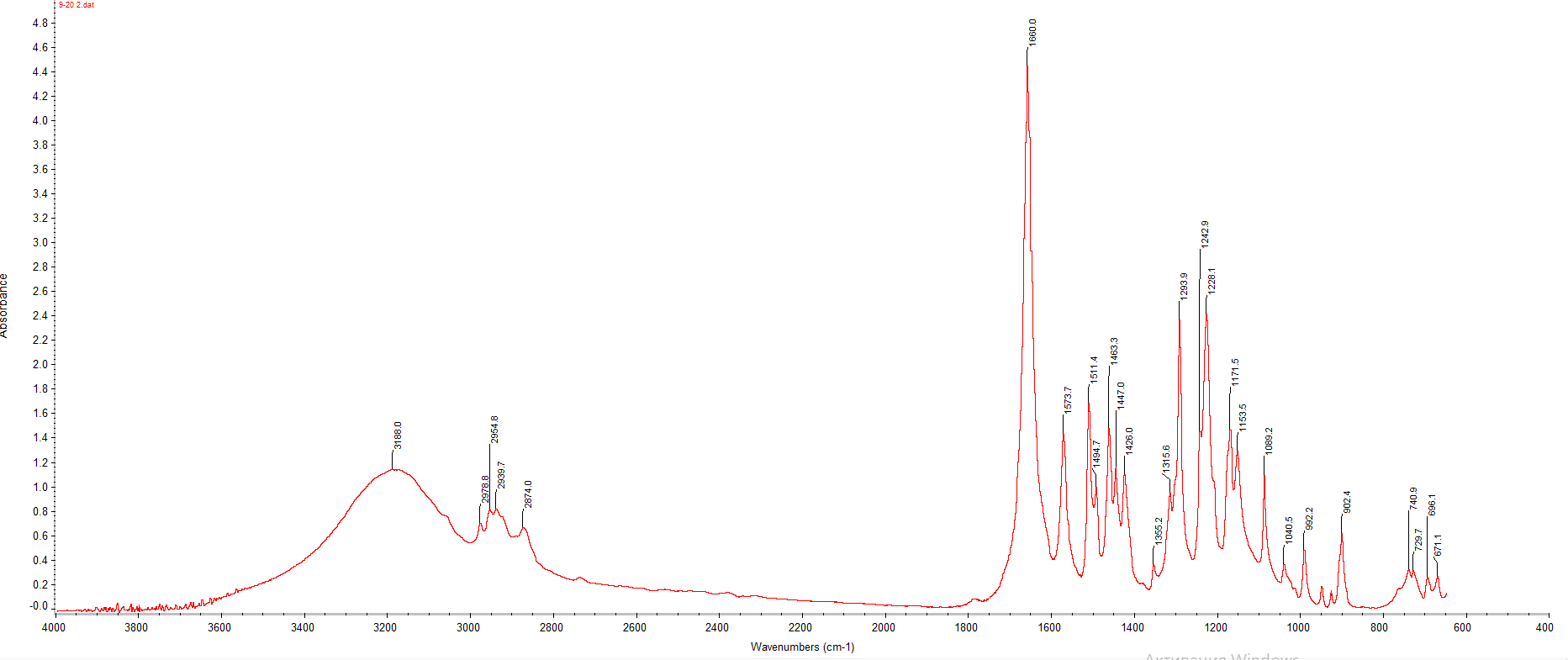
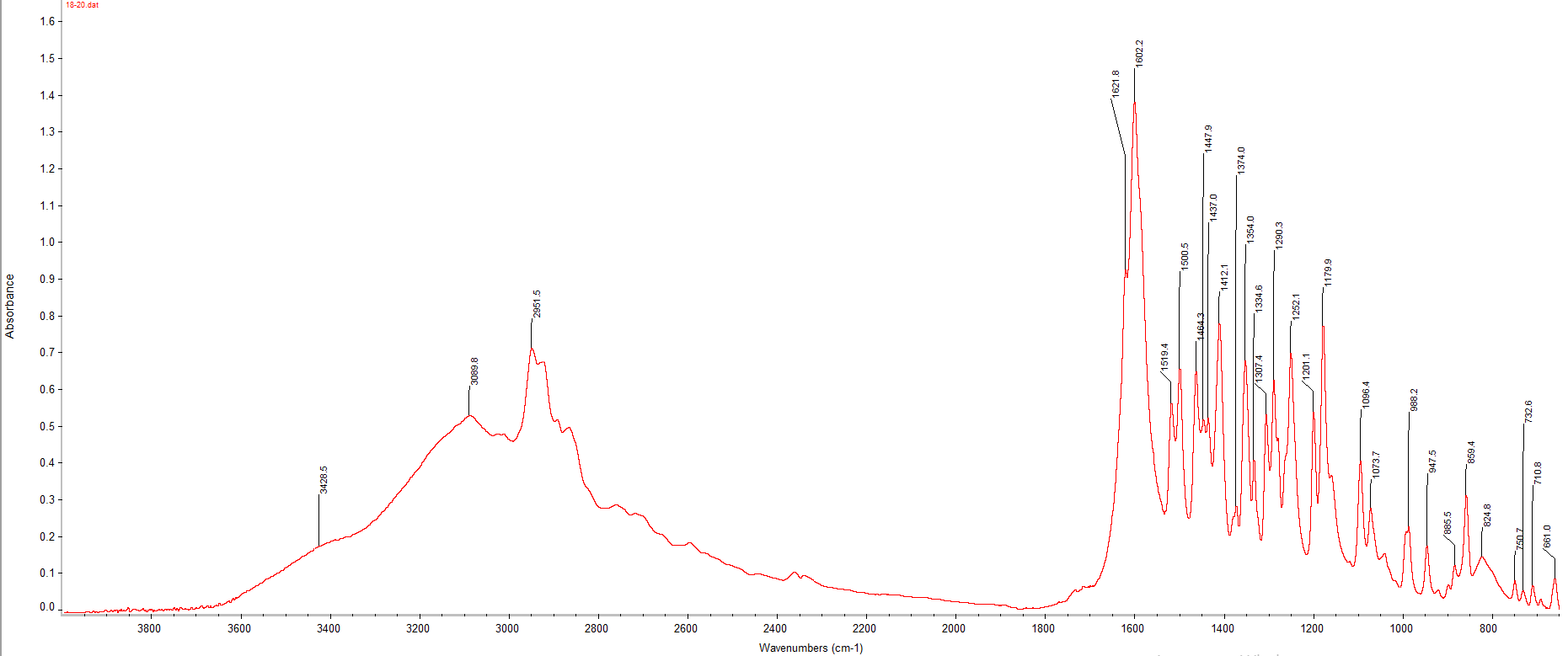
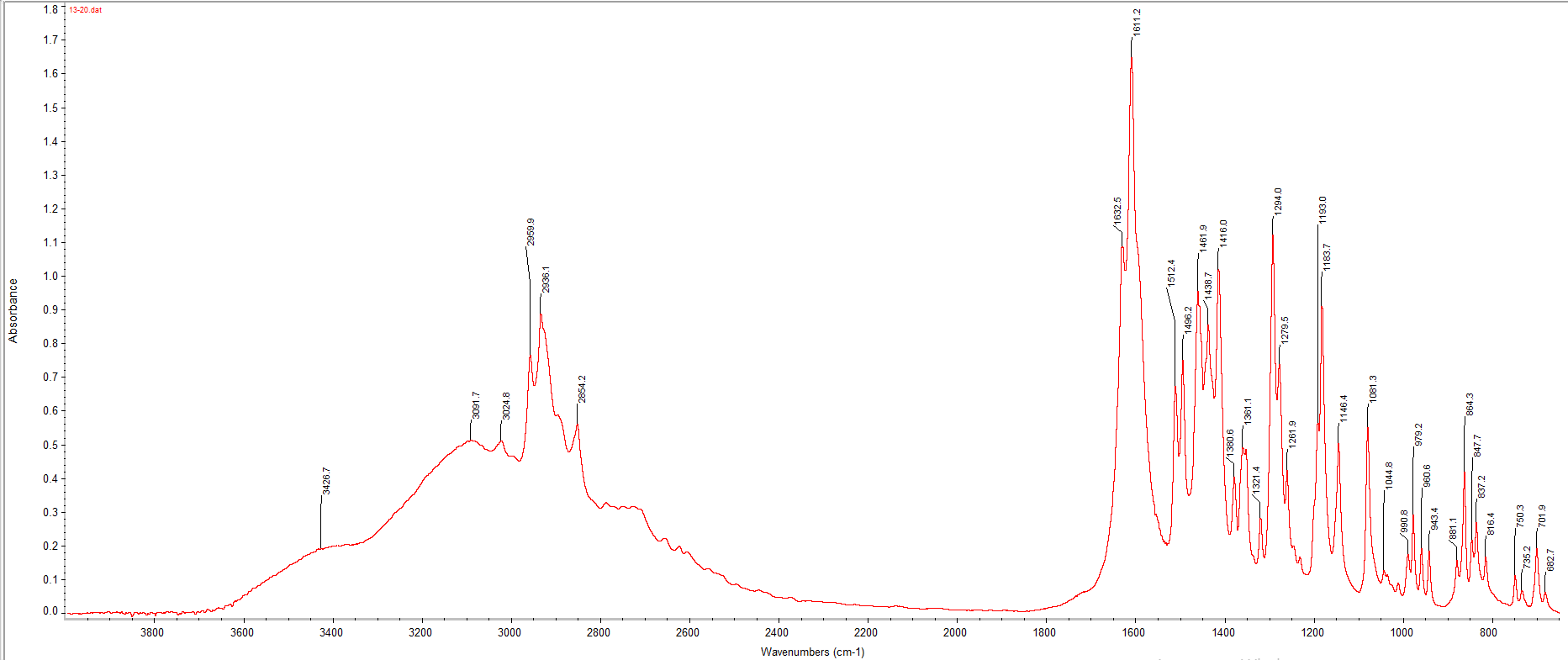
IR spectra of the 1-(4-hydroxy-2,5-dimethylbenzyl)pyrrolidin-2-one (3)



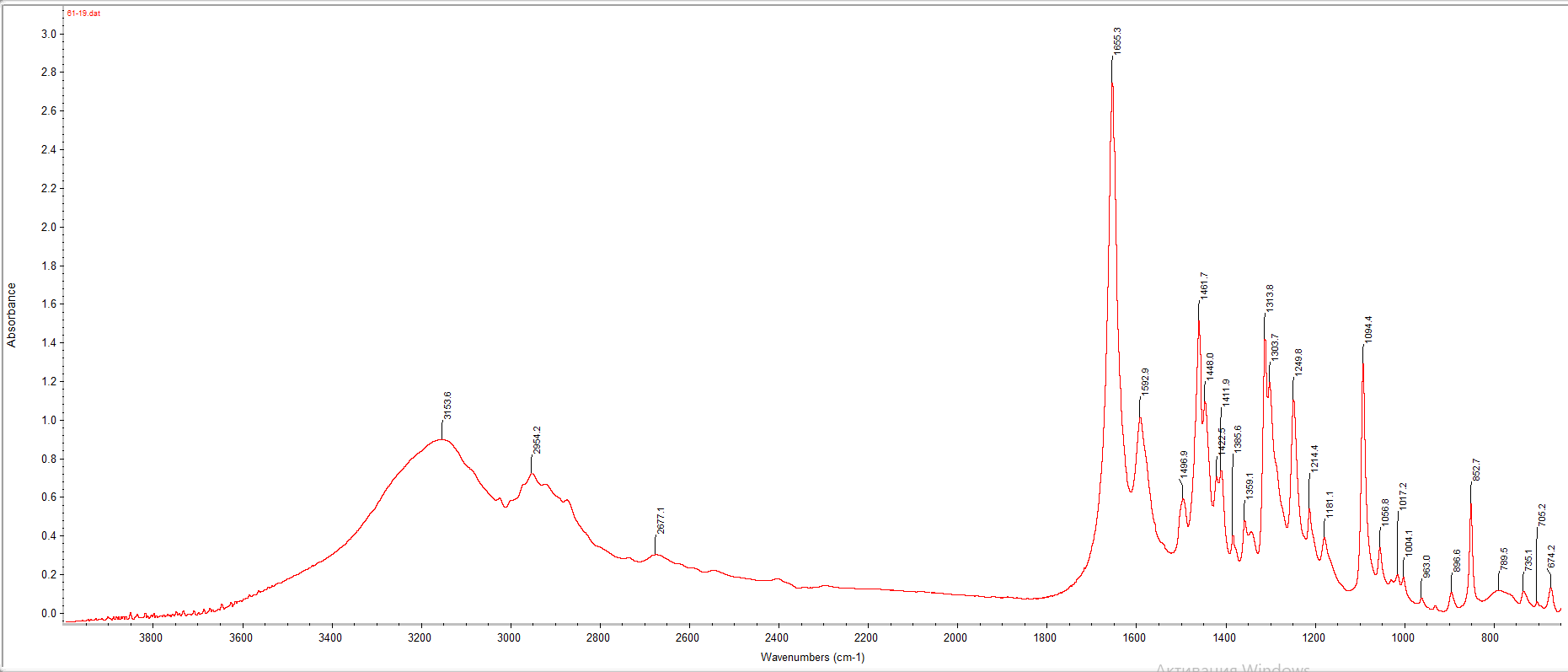
IR spectra of the 1-(4-hydroxy-2,5-dimethylbenzyl)piperidin-2-one (4)



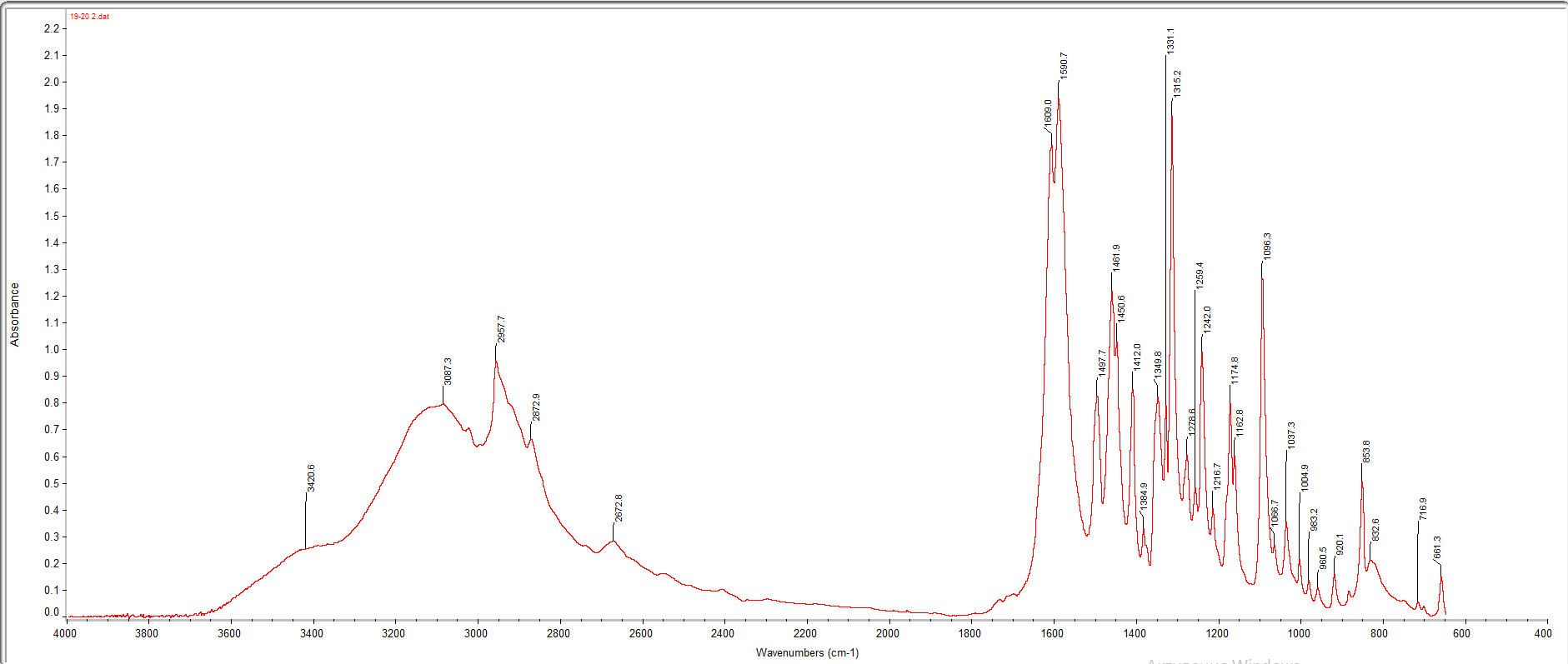
IR spectra of the 1-(4-hydroxy-2,5-dimethylbenzyl)azepan-2-one(**5**)



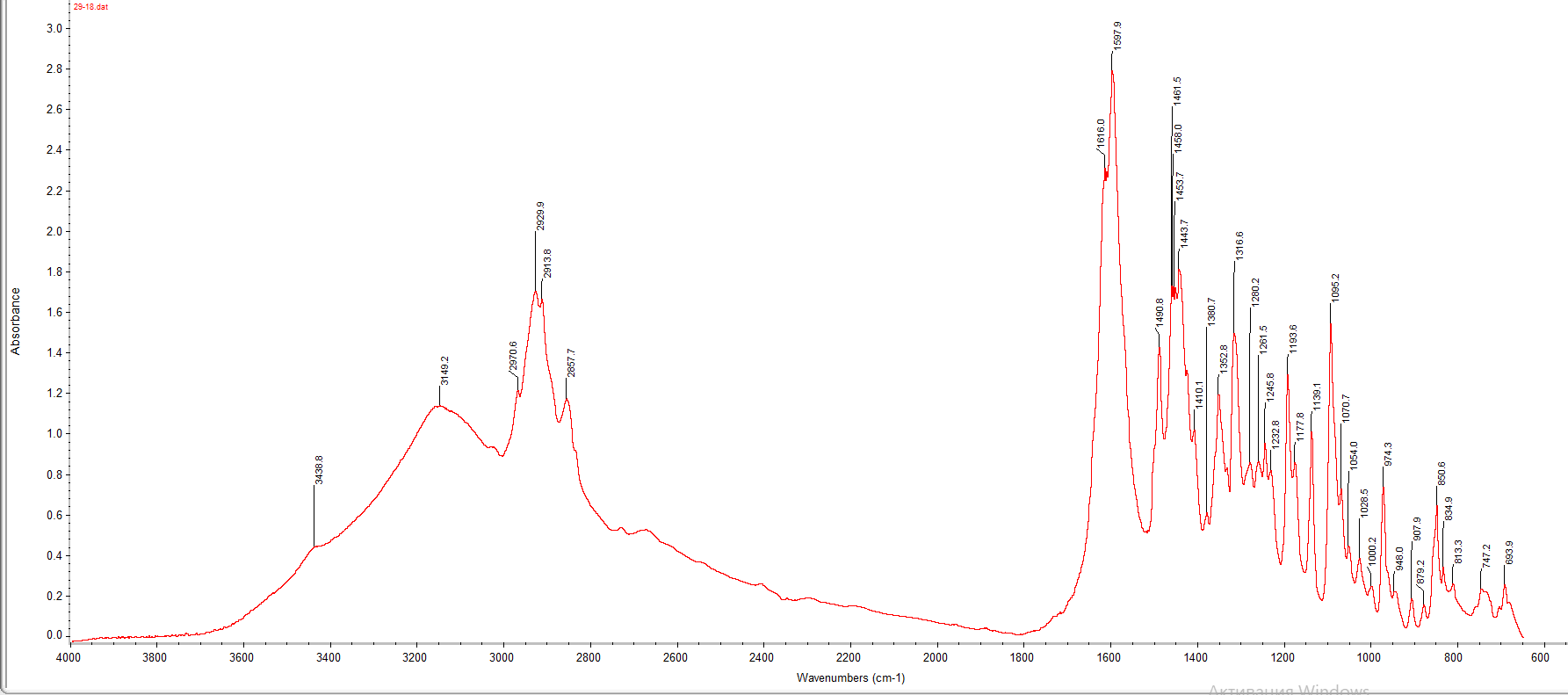
IR spectra of the 1-(4-hydroxy-2,3,6-trimethylbenzyl)pyrrolidin-2-one (6)



IR spectra of the 1-(4-hydroxy-2,3,6-trimethylbenzyl)piperidin-2-one(**7**)

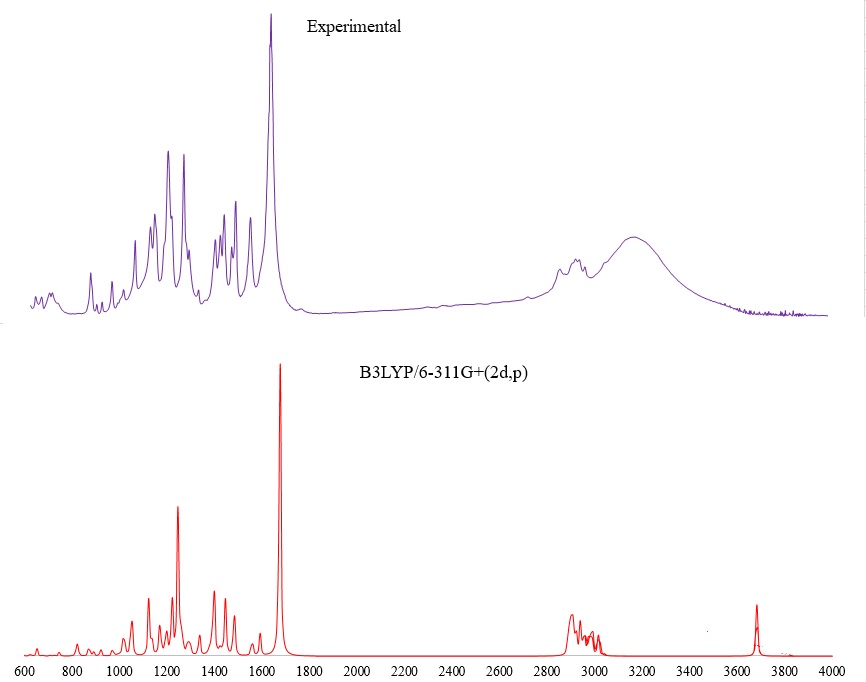


IR spectra of the 1-(4-hydroxy-2,3,6-trimethylbenzyl)azepan-2-one (8)

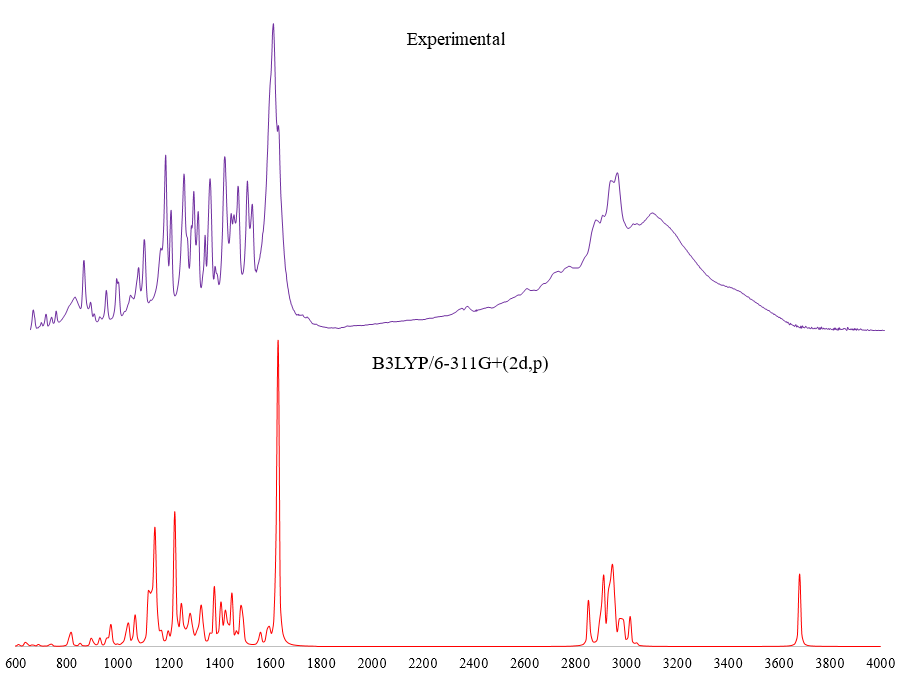


The experimental and calculated (B3LYP/6-311G+(2d,p)) IR spectra

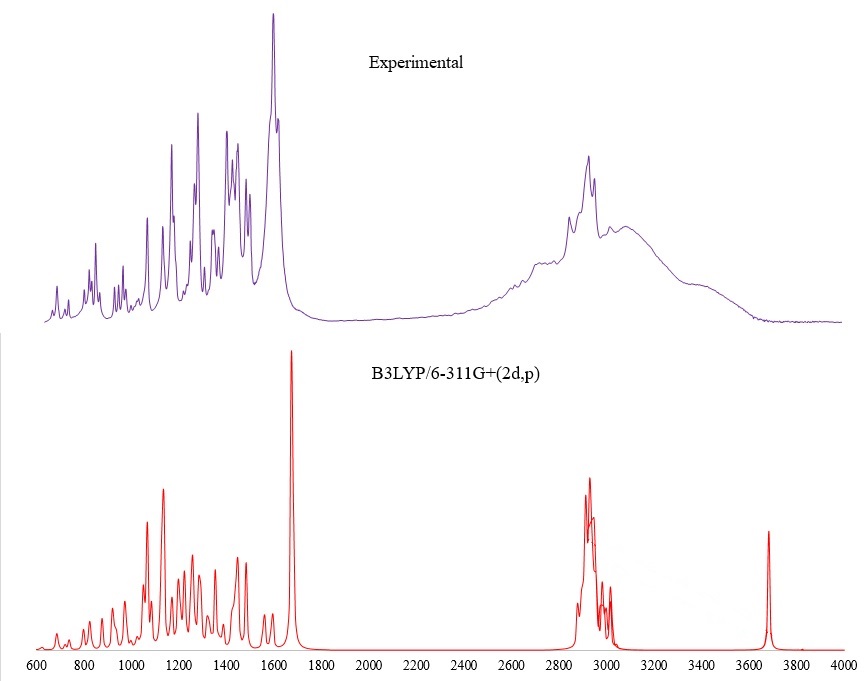
1-(4-hydroxy-2,5-dimethylbenzyl)pyrrolidin-2-one (**3**)



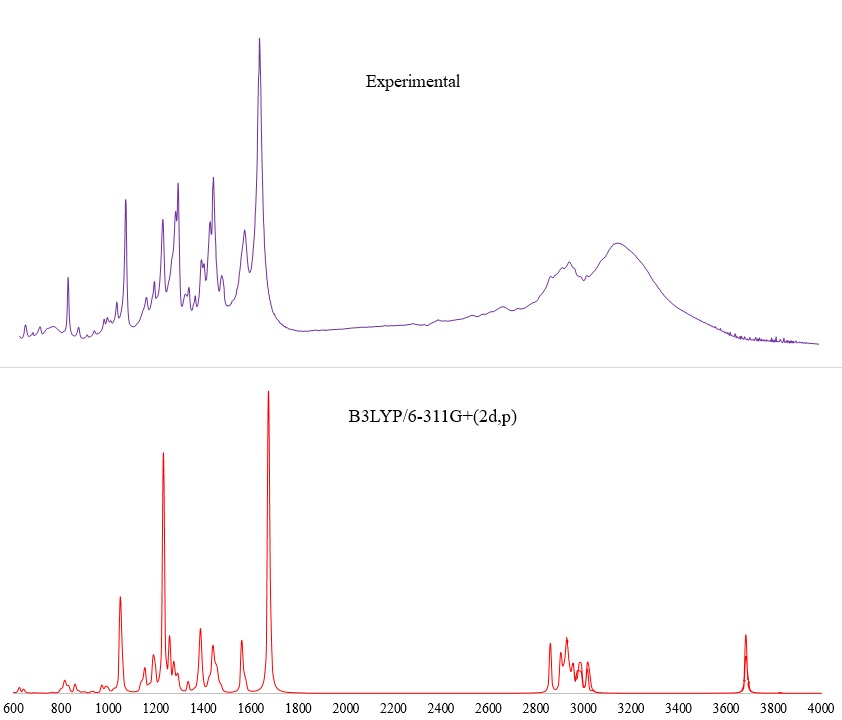
1-(4-hydroxy-2,5-dimethylbenzyl)piperidin-2-one(**4**)



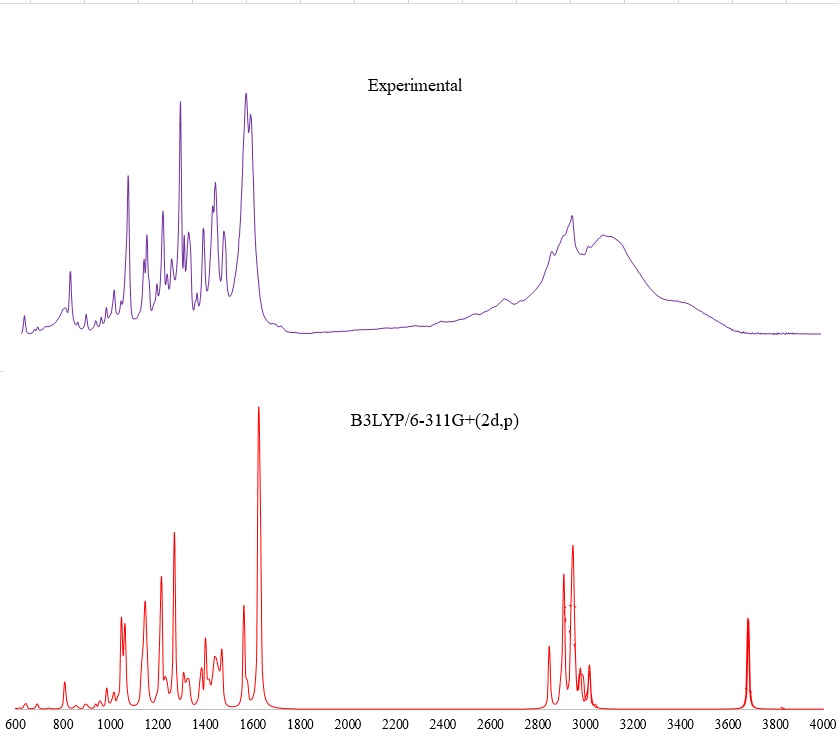
1-(4-hydroxy-2,5-dimethylbenzyl)azepan-2-one(**5**)



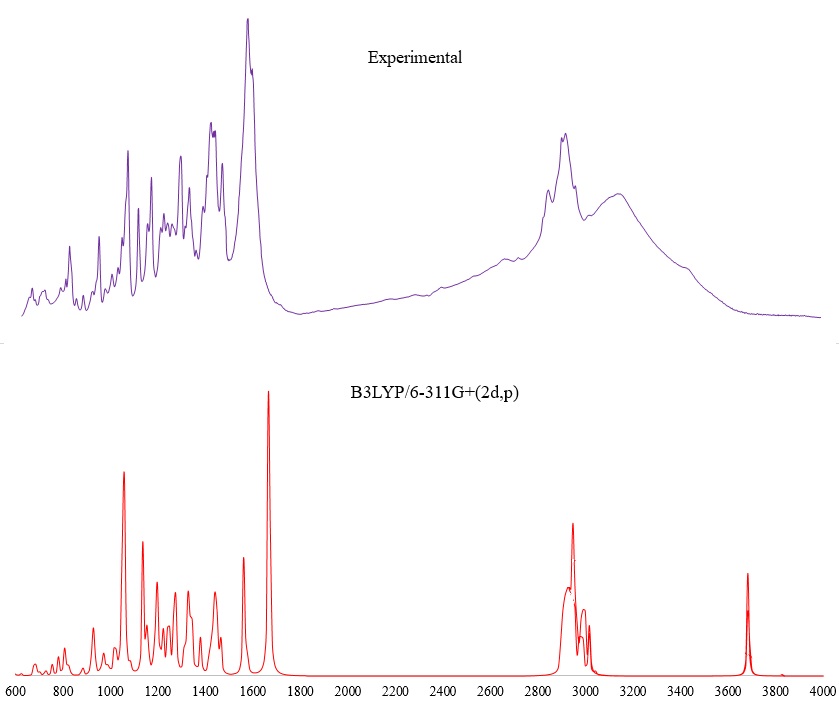
1-(4-hydroxy-2,3,6-trimethylbenzyl)pyrrolidin-2-one(**6**)



1-(4-hydroxy-2,3,6-trimethylbenzyl)piperidin-2-one(**7**)



1-(4-hydroxy-2,3,6-trimethylbenzyl)azepan-2-one(**8**)



Experimental and calculated wavenumbers of FT-IR spectra of compound **3** by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | IR calculated, scaled ν(cm-1) | IR calculated, unscaled ν(cm-1 | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % |
| 3186 | 3680.222 | 3828.38 | s1 | 100 |  |  |  |  |
| 3030 | 3021.952 | 3143.61 | s2 | 98 |  |  |  |  |
| 3022 | 3011.465 | 3132.7 | s3 | 98 |  |  |  |  |
| 3003 | 2991.018 | 3111.43 | s15 | 81 |  |  |  |  |
| - | 2990.518 | 3110.91 | s7 | -96 |  |  |  |  |
| 2982 | 2982.414 | 3102.48 | s5 | -21 | s6 | 78 |  |  |
| 2978 | 2978.838 | 3098.76 | s14 | -80 | s15 | -10 |  |  |
| - | 2968.273 | 3087.77 | s10 | 92 |  |  |  |  |
| - | 2959.429 | 3078.57 | s8 | -96 |  |  |  |  |
| 2955 | 2952.518 | 3071.38 | s4 | 100 |  |  |  |  |
| 2939 | 2939.348 | 3057.68 | s13 | 10 | s16 | 66 |  |  |
| 2924 | 2924.909 | 3042.66 | s16 | -13 | s17 | 80 |  |  |
| - | 2921.804 | 3039.43 | s13 | -78 | s16 | 11 |  |  |
| - | 2909.624 | 3026.76 | s5 | 77 | s6 | 21 |  |  |
| - | 2909.125 | 3026.24 | s9 | 96 |  |  |  |  |
| 2895 | 2899.137 | 3015.85 | s11 | 90 |  |  |  |  |
| 2874 | 2888.793 | 3005.09 | s12 | 86 |  |  |  |  |
| 1660 | 1674.806 | 1742.23 | s18 | 83 |  |  |  |  |
| 1573 | 1591.701 | 1655.78 | s20 | 57 | s36 | -14 |  |  |
| 1512 | 1557.796 | 1620.51 | s22 | 51 | s33 | 10 |  |  |
| 1494 | 1484.363 | 1544.12 | s37 | 38 |  |  |  |  |
| 1471 | 1477.018 | 1536.48 | s47 | 77 |  |  |  |  |
| 1458 | 1446.814 | 1505.06 | s49 | 81 |  |  |  |  |
| 1446 | 1445.805 | 1504.01 | s41 | 62 | s67 | -14 |  |  |
| - | 1444.228 | 1502.37 | s45 | 71 | s72 | 11 |  |  |
| - | 1433.789 | 1491.51 | s39 | 67 |  |  |  |  |
| 1425 | 1425.819 | 1483.22 | s42 | -69 |  |  |  |  |
| - | 1422.676 | 1479.95 | s38 | -77 | s68 | 13 |  |  |
| 1413 | 1417.677 | 1474.75 | s51 | 84 |  |  |  |  |
| - | 1397.105 | 1453.35 | s24 | 20 | s75 | -12 | s76 | 11 |
| 1381 | 1381.167 | 1436.77 | s21 | 23 |  |  |  |  |
| 1367 | 1367.276 | 1422.32 | s43 | 75 |  |  |  |  |
| 1356 | 1363.604 | 1418.5 | s40 | 83 |  |  |  |  |
| - | 1336.082 | 1389.87 | s73 | 48 |  |  |  |  |
| - | 1298.091 | 1350.35 | s19 | 12 | s73 | 10 | s77 | 10 |
| - | 1289.738 | 1341.66 | s19 | -19 | s48 | 11 | s77 | 16 |
| - | 1284.133 | 1335.83 | s35 | -13 | s36 | -20 |  |  |
| 1315 | 1264.821 | 1315.74 | s19 | 24 | s25 | -10 | s36 | -12 |
| 1305 | 1257.371 | 1307.99 | s48 | -19 | s80 | -51 |  |  |
| 1294 | 1245.883 | 1296.04 | s23 | -11 | s25 | 16 | s36 | -15 |
| 1211 | 1221.024 | 1270.18 | s29 | 16 | s50 | 14 | s74 | 11 |
| - | 1201.933 | 1250.32 | s26 | 14 | s35 | -14 |  |  |
| 1245 | 1196.77 | 1244.95 | s50 | 32 |  |  |  |  |
| 1226 | 1177.814 | 1225.23 | s78 | 40 | s80 | -11 |  |  |
| 1211 | 1170.027 | 1217.13 | s28 | -10 | s37 | 38 |  |  |
| - | 1165.807 | 1212.74 | s30 | -16 | s44 | 17 |  |  |
| 1178 | 1136.285 | 1182.03 | s35 | 10 | s46 | 11 | s75 | 13 |
| 1170 | 1123.404 | 1168.63 | s35 | 24 |  |  |  |  |
| 1089 | 1053.412 | 1095.82 | s46 | 21 |  |  |  |  |
| - | 1048.788 | 1091.01 | s27 | 10 | s46 | -16 |  |  |
| - | 1024.39 | 1065.63 | s38 | 21 | s68 | -54 |  |  |
| - | 1018.92 | 1059.94 | s29 | -12 | s31 | 15 | s44 | 12 |
| - | 1013.095 | 1053.88 | s72 | 58 |  |  |  |  |
| 1039 | 996.8296 | 1036.96 | s39 | 11 | s70 | 29 |  |  |
| 1028 | 988.4279 | 1028.22 | s32 | 36 | s34 | -14 | s63 | 11 |
| 1017 | 971.6917 | 1010.81 | s41 | 17 | s67 | -38 |  |  |
| 999 | 921.2042 | 958.29 | s30 | -11 | s74 | -25 |  |  |
| 927 | 891.375 | 927.26 | s32 | 21 | s62 | 18 | s63 | 19 |
| 908 | 873.0527 | 908.2 | s65 | -69 |  |  |  |  |
| 902 | 869.3613 | 904.36 | s34 | 10 | s75 | -14 | s76 | -25 |
| - | 826.122 | 859.38 | s24 | -19 | s48 | -11 | s62 | -12 |
| - | 820.508 | 853.54 | s66 | -71 |  |  |  |  |
| - | 796.5716 | 828.64 | s25 | -13 | s26 | -13 | s28 | 15 |
| 763 | 747.5549 | 777.65 | s61 | 20 | s91 | -12 |  |  |
| 740 | 726.3006 | 755.54 | s23 | 16 | s54 | 15 | s59 | -10 |
| 729 | 708.0647 | 736.57 | s82 | 15 |  |  |  |  |
| 696 | 679.5141 | 706.87 | s26 | -10 | s82 | -16 |  |  |
| 671 | 653.2322 | 679.53 | s63 | 22 |  |  |  |  |
| - | 626.0082 | 651.21 | s34 | 19 | s88 | -21 | s90 | 12 |
| - | 591.411 | 615.22 | s31 | -13 | s62 | 10 | s90 | 31 |
| - | 560.6975 | 583.27 | s58 | 15 | s88 | -14 | s90 | 10 |
| - | 539.6738 | 561.4 | s58 | 29 | s88 | 24 |  |  |
| - | 510.1235 | 530.66 | s58 | 18 | s59 | 10 |  |  |
| - | 478.91 | 498.19 | s52 | 45 |  |  |  |  |
| - | 444.236 | 462.12 | s92 | -66 |  |  |  |  |
| - | 431.9505 | 449.34 | s53 | -11 | s54 | 21 |  |  |
| - | 355.7195 | 370.04 | s93 | 55 |  |  |  |  |
| - | 336.3877 | 349.93 | s57 | 54 | s74 | 13 |  |  |
| - | 317.8731 | 330.67 | s64 | 82 |  |  |  |  |
| - | 303.1171 | 315.32 | s55 | 64 | s59 | -10 |  |  |
| - | 277.4792 | 288.65 | s60 | -66 |  |  |  |  |
| - | 252.2163 | 262.37 | s89 | 49 |  |  |  |  |
| - | 229.2316 | 238.46 | s61 | -13 | s89 | -18 |  |  |
| - | 190.3662 | 198.03 | s56 | 58 |  |  |  |  |
| - | 170.0828 | 176.93 | s87 | 66 |  |  |  |  |
| - | 143.4356 | 149.21 | s86 | 59 |  |  |  |  |
| - | 137.2448 | 142.77 | s77 | -13 | s81 | -38 |  |  |
| - | 126.1706 | 131.25 | s70 | 10 | s71 | 62 |  |  |
| - | 121.6525 | 126.55 | s68 | 13 | s69 | 64 |  |  |
| - | 103.8396 | 108.02 | s82 | -23 | s83 | 49 |  |  |
| - | 58.23555 | 60.58 | s84 | 61 |  |  |  |  |
| - | 43.89296 | 45.66 | s61 | -16 | s84 | 10 | s91 |  |
| - | 31.44412 | 32.71 | \* | 33.47 | s84 | 16 | s85 |  |

Scaling factor = 0.9613, (-)PED% - asymmetric vibrations

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| s 1 | 1.00 | STRE | 16 | 17 | OH | 0.963798 | f3828 100 |  |  |  |
| s 2 | 1.00 | STRE | 2 | 18 | CH | 1.086069 | f3144 98 |  |  |  |
| s 3 | 1.00 | STRE | 5 | 7 | CH | 1.086995 | f3133 98 |  |  |  |
| s 4 | 1.00 | STRE | 8 | 9 | CH | 1.093211 | f3071 100 |  |  |  |
|  | -1.00 |  | 8 | 10 | CH | 1.093192 |  |  |  |  |
| s 5 | 1.00 | STRE | 8 | 9 | CH | 1.093211 | f3102 21 | f3027 77 |  |  |
|  | 1.00 |  | 8 | 10 | CH | 1.093192 |  |  |  |  |
| s 6 | 1.00 | STRE | 8 | 11 | CH | 1.090730 | f3102 78 | f3027 21 |  |  |
| s 7 | 1.00 | STRE | 12 | 13 | CH | 1.090335 | f3111 96 |  |  |  |
|  | -1.00 |  | 12 | 15 | CH | 1.091121 |  |  |  |  |
| s 8 | -1.00 | STRE | 12 | 13 | CH | 1.090335 | f3079 96 |  |  |  |
|  | 1.00 |  | 12 | 14 | CH | 1.094407 |  |  |  |  |
|  | -1.00 |  | 12 | 15 | CH | 1.091121 |  |  |  |  |
| s 9 | 1.00 | STRE | 12 | 13 | CH | 1.090335 | f3026 96 |  |  |  |
|  | 1.00 |  | 12 | 14 | CH | 1.094407 |  |  |  |  |
|  | 1.00 |  | 12 | 15 | CH | 1.091121 |  |  |  |  |
| s 10 | 1.00 | STRE | 19 | 20 | CH | 1.091116 | f3088 92 |  |  |  |
| s 11 | 1.00 | STRE | 19 | 21 | CH | 1.095174 | f3016 90 |  |  |  |
| s 12 | 1.00 | STRE | 22 | 25 | CH | 1.095769 | f3005 86 |  |  |  |
| s 13 | 1.00 | STRE | 22 | 26 | CH | 1.093365 | f3058 10 | f3039 78 |  |  |
|  | -1.00 |  | 27 | 31 | CH | 1.094294 |  |  |  |  |
| s 14 | 1.00 | STRE | 24 | 28 | CH | 1.091680 | f3099 80 |  |  |  |
|  | -1.00 |  | 24 | 29 | CH | 1.089706 |  |  |  |  |
|  | -1.00 |  | 27 | 30 | CH | 1.089123 |  |  |  |  |
| s 15 | 1.00 | STRE | 24 | 28 | CH | 1.091680 | f3111 81 | f3099 10 |  |  |
|  | -1.00 |  | 24 | 29 | CH | 1.089706 |  |  |  |  |
|  | 1.00 |  | 27 | 30 | CH | 1.089123 |  |  |  |  |
| s 16 | 1.00 | STRE | 24 | 28 | CH | 1.091680 | f3058 66 | f3043 13 | f3039 11 |  |
| s 17 | 1.00 | STRE | 22 | 26 | CH | 1.093365 | f3043 80 |  |  |  |
|  | 1.00 |  | 27 | 31 | CH | 1.094294 |  |  |  |  |
| s 18 | 1.00 | STRE | 33 | 23 | OC | 1.219245 | f1742 83 |  |  |  |
| s 19 | 1.00 | STRE | 2 | 3 | CC | 1.391162 | f1350 12 | f1342 19 | f1316 23 |  |
|  | 1.00 |  | 4 | 5 | CC | 1.390317 |  |  |  |  |
| s 20 | 1.00 | STRE | 4 | 5 | CC | 1.390317 | f1656 57 |  |  |  |
|  | 1.00 |  | 1 | 2 | CC | 1.396313 |  |  |  |  |
| s 21 | 1.00 | STRE | 1 | 2 | CC | 1.396313 | f1437 23 |  |  |  |
|  | 1.00 |  | 2 | 3 | CC | 1.391162 |  |  |  |  |
| s 22 | 1.00 | STRE | 3 | 4 | CC | 1.396684 | f1621 51 |  |  |  |
|  | -1.00 |  | 5 | 6 | CC | 1.394731 |  |  |  |  |
| s 23 | 1.00 | STRE | 5 | 6 | CC | 1.394731 | f1296 11 | f756 16 |  |  |
|  | 1.00 |  | 3 | 4 | CC | 1.396684 |  |  |  |  |
|  | 1.00 |  | 4 | 5 | CC | 1.390317 |  |  |  |  |
| s 24 | 1.00 | STRE | 32 | 23 | NC | 1.365791 | f1453 21 | f859 18 |  |  |
| s 25 | 1.00 | STRE | 16 | 4 | OC | 1.372469 | f1316 10 | f1296 16 | f829 14 |  |
| s 26 | 1.00 | STRE | 8 | 3 | CC | 1.504398 | f1250 15 | f829 14 | f707 10 |  |
| s 27 | 1.00 | STRE | 12 | 6 | CC | 1.508554 | f1091 10 |  |  |  |
| s 28 | 1.00 | STRE | 19 | 1 | CC | 1.516078 | f1217 10 | f829 16 |  |  |
| s 29 | 1.00 | STRE | 32 | 19 | NC | 1.457108 | f1270 16 | f1060 12 |  |  |
| s 30 | 1.00 | STRE | 32 | 22 | NC | 1.457620 | f1213 15 | f958 11 |  |  |
| s 31 | 1.00 | STRE | 27 | 23 | CC | 1.525503 | f1060 15 | f615 12 |  |  |
| s 32 | 1.00 | STRE | 24 | 27 | CC | 1.534527 | f1028 36 | f927 20 |  |  |
| s 33 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.52 | f1621 10 |  |  |  |  |
| s 34 | 1.00 | BEND | 24 | 27 | 23 | CCC | 104.45 | f1028 14 | f904 10 | f651 17 |  |  |
| s 35 | 1.00 | BEND | 17 | 16 | 4 | HOC | 109.46 | f1342 10 | f1336 1 | 3 f1250 | 14 f1169 24 | |
| s 36 | 1.00 | BEND | 18 | 2 | 1 | HCC | 118.51 | f1656 14 | f1336 2 | 1 f1316 | 12 f1296 15 | |
|  | -1.00 |  | 7 | 5 | 6 | HCC | 119.14 |  |  |  |  |  |
| s 37 | 1.00 | BEND | 7 | 5 | 6 | HCC | 119.14 | f1544 39 | f1217 38 |  |  |  |
|  | 1.00 |  | 18 | 2 | 1 | HCC | 118.51 |  |  |  |  |  |
| s 38 | 1.00 | BEND | 9 | 8 | 11 | HCH | 108.31 | f1480 77 | f1066 21 |  |  |  |
|  | -1.00 |  | 10 | 8 | 11 | HCH | 108.35 |  |  |  |  |  |
| s 39 | -1.00 | BEND | 13 | 12 | 15 | HCH | 108.32 | f1492 67 | f1037 11 |  |  |  |
|  | 1.00 |  | 9 | 8 | 10 | HCH | 106.58 |  |  |  |  |  |
|  | 1.00 |  | 13 | 12 | 14 | HCH | 106.43 |  |  |  |  |  |
| s 40 | 1.00 | BEND | 9 | 8 | 10 | HCH | 106.58 | f1419 83 |  |  |  |  |
|  | 1.00 |  | 9 | 8 | 11 | HCH | 108.31 |  |  |  |  |  |
|  | 1.00 |  | 10 | 8 | 11 | HCH | 108.35 |  |  |  |  |  |
| s 41 | 1.00 | BEND | 9 | 8 | 10 | HCH | 106.58 | f1504 62 | f1011 17 |  |  |  |
|  | -1.00 |  | 9 | 8 | 11 | HCH | 108.31 |  |  |  |  |  |
|  | 1.00 |  | 14 | 12 | 15 | HCH | 107.36 |  |  |  |  |  |
| s 42 | -1.00 | BEND | 14 | 12 | 15 | HCH | 107.36 | f1483 69 |  |  |  |  |
|  | -1.00 |  | 20 | 19 | 21 | HCH | 107.32 |  |  |  |  |  |
|  | 1.00 |  | 13 | 12 | 15 | HCH | 108.32 |  |  |  |  |  |
| s 43 | 1.00 | BEND | 13 | 12 | 14 | HCH | 106.43 | f1422 75 |  |  |  |  |
|  | 1.00 |  | 14 | 12 | 15 | HCH | 107.36 |  |  |  |  |  |
| s 44 | 1.00 | BEND | 20 | 19 | 1 | HCC | 111.62 | f1213 16 | f1060 13 |  |  |  |
| s 45 | 1.00 | BEND | 20 | 19 | 21 | HCH | 107.32 | f1502 71 |  |  |  |  |
|  | 1.00 |  | 13 | 12 | 15 | HCH | 108.32 |  |  |  |  |  |
| s 46 | 1.00 | BEND | 25 | 22 | 24 | HCC | 112.13 | f1225 11 | f1182 10 | f1096 19 | f1091 15 |  |
|  | -1.00 |  | 30 | 27 | 23 | HCC | 110.28 |  |  |  |  |  |
| s 47 | 1.00 | BEND | 26 | 22 | 25 | HCH | 107.34 | f1536 78 |  |  |  |  |
| s 48 | 1.00 | BEND | 28 | 24 | 27 | HCC | 110.00 | f1342 11 | f1308 20 | f859 10 |  |  |
| s 49 | 1.00 | BEND | 29 | 24 | 28 | HCH | 107.64 | f1505 81 |  |  |  |  |
| s 50 | 1.00 | BEND | 25 | 22 | 24 | HCC | 112.13 | f1270 14 | f1245 32 |  |  |  |
| s 51 | 1.00 | BEND | 31 | 27 | 30 | HCH | 107.35 | f1475 84 |  |  |  |  |
| s 52 | 1.00 | BEND | 33 | 23 | 27 | OCC | 126.52 | f498 45 |  |  |  |  |
| s 53 | 1.00 | BEND | 5 | 4 | 3 | CCC | 120.85 | f449 11 |  |  |  |  |
| s 54 | 1.00 | BEND | 4 | 3 | 2 | CCC | 116.78 | f756 15 | f449 21 |  |  |  |
| s 55 | 1.00 | BEND | 5 | 6 | 12 | CCC | 119.26 | f315 64 |  |  |  |  |
|  | 1.00 |  | 5 | 4 | 16 | CCO | 121.97 |  |  |  |  |  |
| s 56 | 1.00 | BEND | 19 | 32 | 23 | CNC | 123.07 | f198 58 |  |  |  |  |
|  | -1.00 |  | 6 | 1 | 19 | CCC | 122.27 |  |  |  |  |  |
| s 57 | 1.00 | BEND | 19 | 32 | 23 | CNC | 123.07 | f350 54 |  |  |  |  |
|  | 1.00 |  | 6 | 1 | 19 | CCC | 122.27 |  |  |  |  |  |
|  | 1.00 |  | 5 | 4 | 16 | CCO | 121.97 |  |  |  |  |  |
| s 58 | -1.00 | BEND | 6 | 1 | 19 | CCC | 122.27 | f583 15 | f561 30 | f531 18 |  |  |
|  | 1.00 |  | 5 | 4 | 16 | CCO | 121.97 |  |  |  |  |  |
|  | -1.00 |  | 5 | 6 | 12 | CCC | 119.26 |  |  |  |  |  |
|  | 1.00 |  | 4 | 3 | 8 | CCC | 120.77 |  |  |  |  |  |
| s 59 | 1.00 | BEND | 4 | 5 | 6 | CCC | 121.81 | f756 10 | f531 10 | f315 10 |  |  |
| s 60 | 1.00 | BEND | 4 | 3 | 8 | CCC | 120.77 | f289 66 |  |  |  |  |
|  | -1.00 |  | 5 | 4 | 16 | CCO | 121.97 |  |  |  |  |  |
| s 61 | 1.00 | BEND | 32 | 19 | 1 | NCC | 114.59 | f778 20 | f238 11 | f46 16 |  |  |
| s 62 | 1.00 | BEND | 22 | 32 | 23 | CNC | 114.11 | f927 17 | f859 12 | f615 10 |  |  |
| s 63 | 1.00 | BEND | 27 | 23 | 32 | CCN | 107.68 | f1028 11 | f927 18 | f680 21 |  |  |
| s 64 | 1.00 | TORS | 17 | 16 | 4 | 3 | HOCC | -179.31 | f331 82 |  |  |  |
| s 65 | 1.00 | TORS | 18 | 2 | 1 | 19 | HCCC | 0.20 | f908 69 |  |  |  |
| s 66 | 1.00 | TORS | 7 | 5 | 6 | 12 | HCCC | 11324,00 | f854 69 |  |  |  |
| s 67 | 1.00 | TORS | 9 | 8 | 3 | 2 | HCCC | -120.18 | f1504 14 | f1060 11 | f1011 38 |  |
|  | -1.00 |  | 10 | 8 | 3 | 2 | HCCC | -238.95 |  |  |  |  |
| s 68 | 1.00 | TORS | 11 | 8 | 3 | 2 | HCCC | 0.39 | f1480 13 | f1066 53 | f126 13 |  |
| s 69 | 1.00 | TORS | 9 | 8 | 3 | 2 | HCCC | -120.18 | f126 65 |  |  |  |
|  | 1.00 |  | 10 | 8 | 3 | 2 | HCCC | -238.95 |  |  |  |  |
| s 70 | 1.00 | TORS | 14 | 12 | 6 | 5 | HCCC | -262.20 | f1037 30 | f131 10 |  |  |
| s 71 | 1.00 | TORS | 14 | 12 | 6 | 5 | HCCC | -262.20 | f131 62 |  |  |  |
|  | 1.00 |  | 13 | 12 | 6 | 5 | HCCC | -142.90 |  |  |  |  |
|  | 1.00 |  | 15 | 12 | 6 | 5 | HCCC | -21.47 |  |  |  |  |
| s 72 | -1.00 | TORS | 15 | 12 | 6 | 5 | HCCC | -21.47 | f1502 11 | f1054 58 |  |  |
|  | 1.00 |  | 13 | 12 | 6 | 5 | HCCC | -142.90 |  |  |  |  |
| s 73 | 1.00 | TORS | 20 | 19 | 1 | 2 | HCCC | -231.10 | f1390 48 | f1350 11 |  |  |
|  | -1.00 |  | 21 | 19 | 1 | 2 | HCCC | 10.75 |  |  |  |  |
| s 74 | 1.00 | TORS | 21 | 19 | 1 | 2 | HCCC | 10.75 | f1270 11 | f958 25 | f350 13 |  |
| s 75 | 1.00 | TORS | 25 | 22 | 32 | 19 | HCNC | -71.95 | f1453 13 | f1182 12 | f904 14 |  |
| s 76 | 1.00 | TORS | 26 | 22 | 32 | 19 | HCNC | 46.90 | f904 22 |  |  |  |
| s 77 | 1.00 | TORS | 28 | 24 | 27 | 23 | HCCC | -265.80 | f1350 11 | f1342 16 | f859 10 | f143 12 |
| s 78 | 1.00 | TORS | 29 | 24 | 27 | 23 | HCCC | -145.16 | f1225 39 | f859 11 |  |  |
|  | 1.00 |  | 30 | 27 | 23 | 32 | HCCN | -221.74 |  |  |  |  |
| s 79 | -1.00 | TORS | 26 | 22 | 32 | 19 | HCNC | 46.90 | f1213 10 | f1182 11 | f904 11 |  |
|  | 1.00 |  | 30 | 27 | 23 | 32 | HCCN | -221.74 |  |  |  |  |
| s 80 | 1.00 | TORS | 31 | 27 | 23 | 32 | HCCN | -104.82 | f1308 43 |  |  |  |
|  | 1.00 |  | 29 | 24 | 27 | 23 | HCCC | -145.16 |  |  |  |  |
|  | -1.00 |  | 30 | 27 | 23 | 32 | HCCN | -221.74 |  |  |  |  |
| s 81 | 1.00 | OUT | 22 | 19 | 23 | 32 | CCCN | 14.94 | f143 36 |  |  |  |
|  | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | 0.15 |  |  |  |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
|  | -1.00 |  | 19 | 32 | 23 | 27 | CNCC | -182.53 |  |  |  |  |
|  | -1.00 |  | 24 | 27 | 23 | 32 | CCCN | 14.94 |  |  |  |  |
| s 82 | -1.00 | OUT | 12 | 1 | 5 | 6 | CCCC | 0.62 | f737 18 | f707 16 | f238 10 | f108 22 |
|  | -1.00 |  | 22 | 19 | 23 | 32 | CCCN | 2.45 |  |  |  |  |
|  | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | 0.00 |  |  |  |  |
|  | 1.00 | OUT | 16 | 3 | 5 | 4 | OCCC | 0.29 |  |  |  |  |
| s 83 | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | 0.15 | f238 10 | f108 46 |  |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
|  | 1.00 |  | 19 | 32 | 23 | 27 | CNCC | -182.53 |  |  |  |  |
|  | 1.00 |  | 24 | 27 | 23 | 32 | CCCN | 14.94 |  |  |  |  |
| s 84 | 1.00 | TORS | 23 | 32 | 19 | 1 | CNCC | -121.46 | f61 62 | f46 10 | f33 15 |  |
| s 85 | 1.00 | TORS | 32 | 19 | 1 | 2 | NCCC | -111.12 | f33 67 |  |  |  |
| s 86 | 1.00 | TORS | 19 | 32 | 23 | 27 | CNCC | -182.53 | f149 60 |  |  |  |
|  | -1.00 |  | 24 | 27 | 23 | 32 | CCCN | 14.94 |  |  |  |  |
| s 87 | 1.00 | OUT | 22 | 19 | 23 | 32 | CCCN | 2.45 | f177 63 |  |  |  |
|  | -1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
|  | 1.00 |  | 24 | 27 | 23 | 32 | CCCN | 14.94 |  |  |  |  |
|  | 1.00 | OUT | 16 | 3 | 5 | 4 | OCCC | 0.29 |  |  |  |  |
| s 88 | 1.00 | OUT | 33 | 27 | 32 | 23 | OCNC | 0.96 | f651 20 | f583 15 | f561 25 |  |
| s 89 | -1.00 | OUT | 8 | 2 | 4 | 3 | CCCC | 0.32 | f262 43 | f238 17 |  |  |
|  | -1.00 |  | 12 | 1 | 5 | 6 | CCCC | 0.62 |  |  |  |  |
|  | -1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | 0.00 |  |  |  |  |
|  | 1.00 |  | 2 | 3 | 4 | 5 | CCCC | 0.15 |  |  |  |  |
|  | -1.00 |  | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
| s 90 | 1.00 | OUT | 12 | 1 | 5 | 6 | CCCC | 0.62 | f680 11 | f651 12 | f615 28 | f583 10 |
|  | 1.00 |  | 16 | 3 | 5 | 4 | OCCC | 0.29 |  |  |  |  |
| s 91 | -1.00 | OUT | 19 | 2 | 6 | 1 | CCCC | 0.74 | f46 39 |  |  |  |
|  | -1.00 |  | 22 | 19 | 23 | 32 | CCCN | 2.45 |  |  |  |  |
|  | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | 0.00 |  |  |  |  |
|  | 1.00 |  | 2 | 3 | 4 | 5 | CCCC | 0.15 |  |  |  |  |
|  | -1.00 |  | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
| s 92 | -1.00 | OUT | 8 | 2 | 4 | 3 | CCCC | 0.32 | f462 63 |  |  |  |
|  | 1.00 |  | 12 | 1 | 5 | 6 | CCCC | 0.62 |  |  |  |  |
|  | 1.00 |  | 19 | 2 | 6 | 1 | CCCC | 0.74 |  |  |  |  |
|  | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | 0.00 |  |  |  |  |
|  | -1.00 |  | 3 | 4 | 5 | 6 | CCCC | -0.23 |  |  |  |  |
|  | -1.00 | OUT | 16 | 3 | 5 | 4 | OCCC | 0.29 |  |  |  |  |
| s 93 | 1.00 | OUT | 8 | 2 | 4 | 3 | CCCC | 0.32 | f370 55 |  |  |  |
|  | 1.00 |  | 12 | 1 | 5 | 6 | CCCC | 0.62 |  |  |  |  |
|  | 1.00 |  | 19 | 2 | 6 | 1 | CCCC | 0.74 |  |  |  |  |
|  | 1.00 |  | 16 | 3 | 5 | 4 | OCCC | 0.29 |  |  |  |  |

Experimental and calculated wavenumbers of FT-IR spectra of compound 4 by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | IR calculated, scaled ν(cm-1) | IR calculated, unscaled ν(cm-1 | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % |
| 3391 | 3829.27 | 3681.077 | s1 | 100 |  |  |  |  |  |  |
| 3028 | 3160.28 | 3037.977 | s2 | 99 |  |  |  |  |  |  |
| 3013 | 3134.74 | 3013.426 | s3 | 99 |  |  |  |  |  |  |
| - | 3107.83 | 2987.557 | s10 | -15 | s11 | 83 |  |  |  |  |
| - | 3105.72 | 2985.529 | s5 | -19 | s6 | 80 |  |  |  |  |
| 2980 | 3097.71 | 2977.829 | s7 | 81 | s9 | -16 |  |  |  |  |
| - | 3090.93 | 2971.311 | s16 | 90 |  |  |  |  |  |  |
| - | 3070.56 | 2951.729 | s4 | -100 |  |  |  |  |  |  |
| - | 3068.56 | 2949.807 | s8 | 98 |  |  |  |  |  |  |
| 2951 | 3067.78 | 2949.057 | s14 | -84 |  |  |  |  |  |  |
| - | 3061.41 | 2942.933 | s18 | 74 | s19 | 11 |  |  |  |  |
| - | 3052.95 | 2934.801 | s10 | 76 | s11 | 14 |  |  |  |  |
| 2928 | 3045.45 | 2927.591 | s13 | 81 |  |  |  |  |  |  |
| - | 3028.24 | 2911.047 | s17 | 79 |  |  |  |  |  |  |
| - | 3026.61 | 2909.48 | s5 | 80 | s6 | 19 |  |  |  |  |
| - | 3023.61 | 2906.596 | s7 | 16 | s9 | 82 |  |  |  |  |
| - | 3021.94 | 2904.991 | s15 | 72 | s19 | -10 |  |  |  |  |
| 2893 | 3012.13 | 2895.561 | s18 | 12 | s19 | 70 |  |  |  |  |
| 2866 | 2966.8 | 2851.985 | s12 | 96 |  |  |  |  |  |  |
| 1622 | 1693.74 | 1628.192 | s20 | 84 |  |  |  |  |  |  |
| 1602 | 1655.65 | 1591.576 | s21 | 61 | s40 | 16 |  |  |  |  |
| 1519 | 1621.47 | 1558.719 | s24 | 49 |  |  |  |  |  |  |
| 1500 | 1546.94 | 1487.073 | s39 | -37 | s58 | 10 |  |  |  |  |
| 1471 | 1527.69 | 1468.568 | s50 | 68 | s82 | -10 |  |  |  |  |
| 1468 | 1507.11 | 1448.785 | s46 | 42 | s73 | 19 |  |  |  |  |
| 1464 | 1505.23 | 1446.978 | s56 | 66 |  |  |  |  |  |  |
| - | 1497.44 | 1439.489 | s48 | 65 |  |  |  |  |  |  |
| - | 1492.81 | 1435.038 | s41 | 54 | s77 | 19 |  |  |  |  |
| - | 1491.48 | 1433.76 | s52 | 80 |  |  |  |  |  |  |
| 1448 | 1483.82 | 1426.396 | s45 | 56 |  |  |  |  |  |  |
| 1444 | 1480.64 | 1423.339 | s43 | 75 | s74 | -23 |  |  |  |  |
| 1437 | 1475.98 | 1418.86 | s45 | 20 | s54 | -27 | s82 | -11 |  |  |
| 1411 | 1460.33 | 1403.815 | s54 | 47 | s82 | -11 |  |  |  |  |
| 1383 | 1434.63 | 1379.11 | s22 | -41 | s46 | 10 |  |  |  |  |
| 1357 | 1419.1 | 1364.181 | s42 | 90 |  |  |  |  |  |  |
| 1354 | 1415.86 | 1361.066 | s44 | 84 |  |  |  |  |  |  |
| 1336 | 1388.35 | 1334.621 | s83 | 59 |  |  |  |  |  |  |
| 1334 | 1386.51 | 1332.852 | s88 | -55 |  |  |  |  |  |  |
| 1325 | 1379.61 | 1326.219 | s49 | 13 | s87 | -42 |  |  |  |  |
| 1309 | 1368.1 | 1315.155 | s47 | 10 | s51 | -13 | s87 | -14 |  |  |
| 1307 | 1357.74 | 1305.195 | s55 | 18 | s86 | 24 |  |  |  |  |
| 1290 | 1339.49 | 1287.652 | s25 | 36 | s38 | -17 |  |  |  |  |
| 1208 | 1323.76 | 1272.53 | s40 | 31 |  |  |  |  |  |  |
| 1265 | 1312.27 | 1261.485 | s49 | 36 |  |  |  |  |  |  |
| 1251 | 1301.71 | 1251.334 | s23 | -13 | s27 | 12 |  |  |  |  |
| - | 1285.75 | 1235.991 | s53 | 44 | s85 | 13 | s86 | 11 |  |  |
| - | 1272.06 | 1222.831 |  |  |  |  |  |  |  |  |
| 1209 | 1245.07 | 1196.886 | s28 | 15 | s38 | -21 | s40 | -17 |  |  |
| 1207 | 1216.29 | 1169.22 | s29 | -12 | s30 | -11 | s39 | 45 |  |  |
| - | 1201.59 | 1155.088 |  |  |  |  |  |  |  |  |
| 1201 | 1192.49 | 1146.341 | s33 | 12 | s35 | 10 | s55 | -15 |  |  |
| 1180 | 1181.59 | 1135.862 | s51 | -19 |  |  |  |  |  |  |
| 1161 | 1168.97 | 1123.731 | s38 | 23 |  |  |  |  |  |  |
| 1103 | 1116.39 | 1073.186 | s55 | -12 | s95 | -11 |  |  |  |  |
| 1095 | 1109.17 | 1066.245 | s32 | 21 |  |  |  |  |  |  |
| 1072 | 1081.22 | 1039.377 | s27 | 10 | s28 | -10 | s29 | -13 | s30 | 12 |
| 1066 | 1073.36 | 1031.821 | s35 | -48 |  |  |  |  |  |  |
| 1060 | 1067.16 | 1025.861 | s43 | 19 | s74 | -60 |  |  |  |  |
| 1043 | 1056.46 | 1015.575 | s45 | 11 | s48 | -12 | s76 | -53 |  |  |
| 1018 | 1037.97 | 997.8006 | s41 | -14 | s77 | -55 |  |  |  |  |
| 955 | 1012.91 | 973.7104 | s46 | 14 | s73 | 48 |  |  |  |  |
| 987 | 998.12 | 959.4928 | s34 | -14 | s68 | 10 |  |  |  |  |
| 922 | 965.86 | 928.4812 | s66 | 12 |  |  |  |  |  |  |
| 900 | 941.66 | 905.2178 | s79 | 15 |  |  |  |  |  |  |
| 885 | 930.5 | 894.4897 | s71 | -67 |  |  |  |  |  |  |
| 860 | 898.57 | 863.7953 | s68 | 11 | s80 | 13 |  |  |  |  |
| 853 | 885.64 | 851.3657 | s34 | 48 |  |  |  |  |  |  |
| 825 | 847.1 | 814.3172 | s72 | 68 | s98 | 13 |  |  |  |  |
| 808 | 844.43 | 811.7506 |  |  |  |  |  |  |  |  |
| 800 | 837.39 | 804.983 | s79 | 10 |  |  |  |  |  |  |
| 750 | 765.26 | 735.6444 | s23 | 27 |  |  |  |  |  |  |
| 732 | 744.49 | 715.6782 | s59 | 12 |  |  |  |  |  |  |
| 711 | 716.99 | 689.2425 | s26 | -12 | s31 | -11 | s33 | -16 | s98 | -18 |
| 692 | 692.2 | 665.4119 | s28 | -14 | s29 | 14 | s59 | 13 | s60 | 10 |
| 659 | 664.62 | 638.8992 | s33 | -10 | s67 | 10 | s79 | -11 | s97 | -13 |
| - | 634.4 | 609.8487 | s91 | 25 | s97 | -13 |  |  |  |  |
| - | 581.16 | 558.6691 | s85 | 20 | s97 | -25 |  |  |  |  |
| - | 560.93 | 539.222 | s64 | 12 | s91 | -14 |  |  |  |  |
| - | 545.12 | 524.0239 | s64 | 36 |  |  |  |  |  |  |
| - | 511.28 | 491.4935 | s57 | 44 |  |  |  |  |  |  |
| - | 483.61 | 464.8943 | s60 | 10 |  |  |  |  |  |  |
| - | 469.62 | 451.4457 | s36 | 10 | s66 | 20 | s68 | -10 |  |  |
| - | 454.89 | 437.2858 | s90 | -62 |  |  |  |  |  |  |
| - | 436.53 | 419.6363 | s36 | 36 | s64 | -16 |  |  |  |  |
| - | 376.27 | 361.7084 | s61 | -15 | s91 | 13 | s102 | 10 |  |  |
| - | 356.78 | 342.9726 | s37 | -25 | s70 | -14 |  |  |  |  |
| - | 330.03 | 317.2578 | s62 | -11 | s70 | 62 |  |  |  |  |
| - | 322.52 | 310.0385 | s62 | 48 | s70 | 14 |  |  |  |  |
| - | 311.9 | 299.8295 | s84 | 23 | s95 | -21 |  |  |  |  |
| - | 291.26 | 279.9882 | s63 | 61 |  |  |  |  |  |  |
| - | 262.94 | 252.7642 | s63 | -12 | s101 | 16 |  |  |  |  |
| - | 250.67 | 240.9691 | s100 | 46 |  |  |  |  |  |  |
| - | 202 | 194.1826 | s61 | -36 | s65 | 27 |  |  |  |  |
| - | 175.98 | 169.1696 | s99 | -50 |  |  |  |  |  |  |
| - | 148.81 | 143.0511 | s76 | 11 | s78 | 64 |  |  |  |  |
| - | 129.38 | 124.373 | s75 | 23 | s93 | 23 |  |  |  |  |
| - | 123.76 | 118.9705 | s75 | 70 | s99 | 11 |  |  |  |  |
| - | 109.07 | 104.849 | s89 | -34 | s94 | -12 | s98 | 13 |  |  |
| - | 96.91 | 93.15958 | s89 | -17 | s94 | 32 |  |  |  |  |
| - | 43.68 | 41.98958 | s69 | 24 | s93 | -17 | s102 | 19 |  |  |
| - | 35.23 | 33.8666 | s92 | 77 |  |  |  |  |  |  |
| - | 18.85 | 18.12051 | s96 | 79 |  |  |  |  |  |  |

Scaling factor = 0.9613, (-)PED% - asymmetric vibrations

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| s 1 | 1.00 | STRE | 34 | 35 | OH | 0.963732 | | f3829 100 | |  | |  | |
| s 2 | 1.00 | STRE | 2 | 7 | CH | 1.085096 | | f3160 99 | |  | |  | |
| s 3 | 1.00 | STRE | 5 | 8 | CH | 1.086771 | | f3135 99 | |  | |  | |
| s 4 | 1.00 | STRE | 9 | 10 | CH | 1.093151 | | f3071 100 | |  | |  | |
|  | -1.00 |  | 9 | 11 | CH | 1.093348 | |  | |  | |  | |
| s 5 | 1.00 | STRE | 9 | 10 | CH | 1.093151 | | f3106 19 | | f3027 80 | |  | |
|  | 1.00 |  | 9 | 11 | CH | 1.093348 | |  | |  | |  | |
| s 6 | 1.00 | STRE | 9 | 12 | CH | 1.090414 | | f3106 80 | | f3027 19 | |  | |
| s 7 | 1.00 | STRE | 13 | 14 | CH | 1.090697 | | f3098 81 | | f3024 16 | |  | |
| s 8 | 1.00 | STRE | 13 | 15 | CH | 1.093458 | | f3069 98 | |  | |  | |
|  | -1.00 |  | 13 | 16 | CH | 1.093255 | |  | |  | |  | |
| s 9 | 1.00 | STRE | 13 | 15 | CH | 1.093458 | | f3098 16 | | f3024 82 | |  | |
|  | 1.00 |  | 13 | 16 | CH | 1.093255 | |  | |  | |  | |
| s 10 | 1.00 | STRE | 17 | 18 | CH | 1.091997 | | f3108 15 | | f3053 76 | |  | |
| s 11 | 1.00 | STRE | 17 | 19 | CH | 1.089278 | | f3108 83 | | f3053 14 | |  | |
| s 12 | 1.00 | STRE | 20 | 23 | CH | 1.099416 | | f2967 96 | |  | |  | |
| s 13 | 1.00 | STRE | 20 | 24 | CH | 1.093468 | | f3045 81 | |  | |  | |
| s 14 | 1.00 | STRE | 22 | 27 | CH | 1.092928 | | f3068 84 | |  | |  | |
|  | -1.00 |  | 22 | 28 | CH | 1.095026 | |  | |  | |  | |
| s 15 | 1.00 | STRE | 22 | 28 | CH | 1.095026 | | f3022 72 | |  | |  | |
|  | 1.00 |  | 22 | 27 | CH | 1.092928 | |  | |  | |  | |
| s 16 | 1.00 | STRE | 25 | 29 | CH | 1.090800 | | f3091 90 | |  | |  | |
| s 17 | 1.00 | STRE | 25 | 30 | CH | 1.095551 | | f3028 79 | |  | |  | |
| s 18 | 1.00 | STRE | 26 | 31 | CH | 1.092902 | | f3061 74 | | f3012 12 | |  | |
| s 19 | 1.00 | STRE | 26 | 32 | CH | 1.095684 | | f3061 11 | | f3022 10 | | f3012 70 | |
|  | 1.00 |  | 26 | 31 | CH | 1.092902 | |  | |  | |  | |
| s 20 | 1.00 | STRE | 36 | 21 | OC | 1.225860 | | f1694 84 | |  | |  | |
| s 21 | 1.00 | STRE | 4 | 5 | CC | 1.388380 | | f1656 61 | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.398343 | |  | |  | |  | |
| s 22 | -1.00 | STRE | 2 | 3 | CC | 1.388952 | | f1435 41 | |  | |  | |
|  | 1.00 |  | 4 | 5 | CC | 1.388380 | |  | |  | |  | |
|  | -1.00 |  | 1 | 2 | CC | 1.398343 | |  | |  | |  | |
| s 23 | 1.00 | STRE | 3 | 4 | CC | 1.398877 | | f1302 13 | | f765 27 | |  | |
|  | 1.00 |  | 2 | 3 | CC | 1.388952 | |  | |  | |  | |
|  | 1.00 |  | 4 | 5 | CC | 1.388380 | |  | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.398343 | |  | |  | |  | |
|  | 1.00 |  | 5 | 6 | CC | 1.397500 | |  | |  | |  | |
| s 24 | 1.00 | STRE | 3 | 4 | CC | 1.398877 | | f1621 50 | |  | |  | |
|  | -1.00 |  | 5 | 6 | CC | 1.397500 | |  | |  | |  | |
| s 25 | 1.00 | STRE | 5 | 6 | CC | 1.397500 | | f1340 37 | |  | |  | |
|  | -1.00 |  | 4 | 5 | CC | 1.388380 | |  | |  | |  | |
|  | -1.00 |  | 2 | 3 | CC | 1.388952 | |  | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.398343 | |  | |  | |  | |
| s 26 | 1.00 | STRE | 33 | 21 | NC | 1.367475 | | f717 12 | |  | |  | |
| s 27 | 1.00 | STRE | 34 | 4 | OC | 1.373181 | | f1302 12 | | f1081 10 | |  | |
| s 28 | 1.00 | STRE | 9 | 3 | CC | 1.504521 | | f1245 16 | | f1081 10 | | f692 15 | |
| s 29 | 1.00 | STRE | 13 | 6 | CC | 1.511973 | | f1216 12 | | f1081 13 | | f692 14 | |
| s 30 | 1.00 | STRE | 17 | 1 | CC | 1.517427 | | f1216 12 | | f1081 12 | |  | |
| s 31 | 1.00 | STRE | 33 | 17 | NC | 1.467582 | | f717 11 | |  | |  | |
|  | 1.00 |  | 21 | 25 | CC | 1.524224 | |  | |  | |  | |
|  | 1.00 |  | 20 | 22 | CC | 1.522043 | |  | |  | |  | |
| s 32 | 1.00 | STRE | 21 | 25 | CC | 1.524224 | | f1109 21 | |  | |  | |
| s 33 | 1.00 | STRE | 33 | 20 | NC | 1.465105 | | f1192 11 | | f717 16 | | f665 10 | |
| s 34 | 1.00 | STRE | 22 | 26 | CC | 1.524807 | | f998 14 | | f886 47 | |  | |
|  | 1.00 |  | 20 | 22 | CC | 1.522043 | |  | |  | |  | |
| s 35 | -1.00 | STRE | 22 | 26 | CC | 1.524807 | | f1192 10 | | f1073 48 | |  | |
|  | 1.00 |  | 20 | 22 | CC | 1.522043 | |  | |  | |  | |
|  | -1.00 |  | 33 | 17 | NC | 1.467582 | |  | |  | |  | |
| s36 | 1.00 | BEND | 2 | 3 | 4 | CCC | 116.97 | | f470 10 | | f437 36 | |  | |
|  | 1.00 |  | 25 | 21 | 36 | CCO | 119.69 | |  | |  | |  | |
|  | -1.00 |  | 20 | 22 | 26 | CCC | 109.98 | |  | |  | |  | |
|  | 1.00 |  | 1 | 2 | 3 | CCC | 123.28 | |  | |  | |  | |
| s 37 | 1.00 | BEND | 20 | 22 | 26 | CCC | 109.98 | | f357 25 | |  | |  | |
|  | -1.00 |  | 17 | 33 | 21 | CNC | 119.14 | |  | |  | |  | |
|  | -1.00 |  | 25 | 21 | 36 | CCO | 119.69 | |  | |  | |  | |
|  | -1.00 |  | 20 | 33 | 21 | CNC | 125.01 | |  | |  | |  | |
| s 38 | 1.00 | BEND | 35 | 34 | 4 | HOC | 109.44 | | f1340 17 | | f1245 21 | | f1169 23 | |
| s 39 | 1.00 | BEND | 8 | 5 | 6 | HCC | 119.26 | | f1547 37 | | f1216 45 | |  | |
|  | 1.00 |  | 7 | 2 | 1 | HCC | 118.29 | |  | |  | |  | |
| s 40 | -1.00 | BEND | 7 | 2 | 1 | HCC | 118.29 | | f1656 16 | | f1324 31 | | f1245 17 | |
|  | 1.00 |  | 8 | 5 | 6 | HCC | 119.26 | |  | |  | |  | |
| s 41 | -1.00 | BEND | 10 | 9 | 11 | HCH | 106.58 | | f1493 54 | | f1038 14 | |  | |
|  | -1.00 |  | 15 | 13 | 16 | HCH | 107.14 | |  | |  | |  | |
|  | 1.00 |  | 14 | 13 | 15 | HCH | 107.43 | |  | |  | |  | |
|  | 1.00 |  | 10 | 9 | 12 | HCH | 108.36 | |  | |  | |  | |
| s 42 | 1.00 | BEND | 10 | 9 | 11 | HCH | 106.58 | | f1419 90 | |  | |  | |
|  | 1.00 |  | 10 | 9 | 12 | HCH | 108.36 | |  | |  | |  | |
|  | 1.00 |  | 11 | 9 | 12 | HCH | 108.44 | |  | |  | |  | |
|  | 1.00 |  | 15 | 13 | 16 | HCH | 107.14 | |  | |  | |  | |
| s 43 | -1.00 | BEND | 10 | 9 | 12 | HCH | 108.36 | | f1481 75 | | f1067 19 | |  | |
|  | 1.00 |  | 11 | 9 | 12 | HCH | 108.44 | |  | |  | |  | |
| s 44 | 1.00 | BEND | 15 | 13 | 16 | HCH | 107.14 | | f1416 84 | |  | |  | |
|  | 1.00 |  | 14 | 13 | 15 | HCH | 107.43 | |  | |  | |  | |
|  | -1.00 |  | 11 | 9 | 12 | HCH | 108.44 | |  | |  | |  | |
|  | -1.00 |  | 10 | 9 | 12 | HCH | 108.36 | |  | |  | |  | |
|  | 1.00 |  | 14 | 13 | 16 | HCH | 107.42 | |  | |  | |  | |
| s 45 | -1.00 | BEND | 14 | 13 | 16 | HCH | 107.42 | | f1484 56 | | f1476 20 | | f1057 11 | |
|  | 1.00 |  | 14 | 13 | 15 | HCH | 107.43 | |  | |  | |  | |
|  | 1.00 |  | 18 | 17 | 19 | HCH | 107.81 | |  | |  | |  | |
| s 46 | -1.00 | BEND | 10 | 9 | 11 | HCH | 106.58 | | f1507 42 | | f1435 10 | | f1013 14 | |
|  | 1.00 |  | 10 | 9 | 12 | HCH | 108.36 | |  | |  | |  | |
| s 47 | 1.00 | BEND | 18 | 17 | 1 | HCC | 110.81 | | f1368 10 | |  | |  | |
| s 48 | 1.00 | BEND | 18 | 17 | 19 | HCH | 107.81 | | f1497 65 | | f1057 12 | |  | |
|  | 1.00 |  | 14 | 13 | 16 | HCH | 107.42 | |  | |  | |  | |
|  | -1.00 |  | 14 | 13 | 15 | HCH | 107.43 | |  | |  | |  | |
| s 49 | 1.00 | BEND | 23 | 20 | 22 | HCC | 109.68 | | f1380 13 | | f1312 36 | |  | |
| s 50 | 1.00 | BEND | 24 | 20 | 23 | HCH | 106.99 | | f1528 68 | |  | |  | |
| s 51 | 1.00 | BEND | 27 | 22 | 26 | HCC | 111.59 | | f1368 13 | | f1182 19 | |  | |
|  | -1.00 |  | 29 | 25 | 26 | HCC | 112.28 | |  | |  | |  | |
| s 52 | 1.00 | BEND | 28 | 22 | 27 | HCH | 107.12 | | f1491 80 | |  | |  | |
| s 53 | 1.00 | BEND | 29 | 25 | 26 | HCC | 112.28 | | f1286 44 | |  | |  | |
|  | 1.00 |  | 27 | 22 | 26 | HCC | 111.59 | |  | |  | |  | |
| s 54 | 1.00 | BEND | 30 | 25 | 29 | HCH | 106.09 | | f1476 27 | | f1460 47 | |  | |
| s 55 | 1.00 | BEND | 31 | 26 | 25 | HCC | 110.24 | | f1358 18 | | f1192 15 | | f1116 12 | |
| s 56 | 1.00 | BEND | 32 | 26 | 31 | HCH | 106.69 | | f1505 66 | |  | |  | |
| s 57 | 1.00 | BEND | 25 | 21 | 36 | CCO | 119.69 | | f511 44 | |  | |  | |
| s 58 | 1.00 | BEND | 5 | 4 | 3 | CCC | 120.84 | | f1547 10 | |  | |  | |
| s 59 | 1.00 | BEND | 2 | 3 | 4 | CCC | 116.97 | | f745 12 | | f692 13 | |  | |
| s 60 | 1.00 | BEND | 6 | 5 | 4 | CCC | 121.63 | | f692 10 | | f484 10 | |  | |
| s 61 | 1.00 | BEND | 2 | 1 | 17 | CCC | 118.28 | | f376 15 | | f202 36 | |  | |
| s 62 | 1.00 | BEND | 5 | 6 | 13 | CCC | 118.89 | | f330 11 | | f323 48 | |  | |
|  | 1.00 |  | 5 | 4 | 34 | CCO | 122.02 | |  | |  | |  | |
| s 63 | 1.00 | BEND | 2 | 3 | 9 | CCC | 122.36 | | f291 61 | | f263 12 | |  | |
|  | 1.00 |  | 5 | 4 | 34 | CCO | 122.02 | |  | |  | |  | |
| s 64 | -1.00 | BEND | 5 | 4 | 34 | CCO | 122.02 | | f561 12 | | f545 36 | | f437 16 | |
|  | 1.00 |  | 5 | 6 | 13 | CCC | 118.89 | |  | |  | |  | |
|  | 1.00 |  | 2 | 3 | 9 | CCC | 122.36 | |  | |  | |  | |
| s 65 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.28 | | f202 27 | |  | |  | |
|  | 1.00 |  | 17 | 33 | 21 | CNC | 119.14 | |  | |  | |  | |
| s 66 | 1.00 | BEND | 22 | 20 | 33 | CCN | 113.38 | | f966 12 | | f470 20 | |  | |
| s 67 | 1.00 | BEND | 25 | 21 | 33 | CCN | 117.97 | | f665 10 | |  | |  | |
| s 68 | 1.00 | BEND | 20 | 22 | 26 | CCC | 109.98 | | f998 10 | | f899 11 | | f470 10 | |
|  | 1.00 |  | 20 | 33 | 21 | CNC | 125.01 | |  | |  | |  | |
|  | -1.00 |  | 25 | 21 | 36 | CCO | 119.69 | |  | |  | |  | |
| s 69 | 1.00 | BEND | 33 | 17 | 1 | NCC | 113.44 | | f44 24 | |  | |  | |
| s 70 | 1.00 | TORS | 35 | 34 | 4 | 3 | HOCC | | -179.05 | | f357 14 | | f330 62 | | f323 14 |
| s 71 | 1.00 | TORS | 7 | 2 | 1 | 17 | HCCC | | 0.18 | | f930 67 | |  | |  |
| s 72 | 1.00 | TORS | 8 | 5 | 6 | 13 | HCCC | | -0.71 | | f847 68 | |  | |  |
| s 73 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.76 | | f1507 19 | | f1013 48 | |  |
|  | -1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.97 | |  | |  | |  |
|  | -1.00 |  | 15 | 13 | 6 | 5 | HCCC | | -116.20 | |  | |  | |  |
|  | 1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -236.58 | |  | |  | |  |
| s 74 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.76 | | f1481 23 | | f1067 60 | |  |
|  | -1.00 |  | 12 | 9 | 3 | 4 | HCCC | | -180.67 | |  | |  | |  |
| s 75 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.76 | | f129 23 | | f124 70 | |  |
|  | 1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.97 | |  | |  | |  |
| s 76 | 1.00 | TORS | 14 | 13 | 6 | 5 | HCCC | | 3.53 | | f1057 53 | | f149 11 | |  |
| s 77 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.76 | | f1493 19 | | f1038 55 | |  |
|  | 1.00 |  | 15 | 13 | 6 | 5 | HCCC | | -116.20 | |  | |  | |  |
|  | -1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.97 | |  | |  | |  |
|  | -1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -236.58 | |  | |  | |  |
| s 78 | 1.00 | TORS | 15 | 13 | 6 | 5 | HCCC | | -116.20 | | f149 64 | |  | |  |
|  | 1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -236.58 | |  | |  | |  |
| s 79 | 1.00 | TORS | 27 | 22 | 26 | 25 | HCCC | | -181.24 | | f942 15 | | f837 10 | | f665 11 |
|  | 1.00 |  | 32 | 26 | 25 | 21 | HCCC | | -74.53 | |  | |  | |  |
|  | 1.00 |  | 31 | 26 | 25 | 21 | HCCC | | -191.97 | |  | |  | |  |
| s 80 | 1.00 | TORS | 19 | 17 | 1 | 6 | HCCC | | -118.21 | | f899 13 | |  | |  |
|  | 1.00 |  | 18 | 17 | 1 | 6 | HCCC | | 1.06 | |  | |  | |  |
| s 81 | 1.00 | TORS | 23 | 20 | 33 | 17 | HCNC | | -70.86 | |  | |  | |  |
| s 82 | 1.00 | TORS | 24 | 20 | 33 | 17 | HCNC | | 44.74 | | f1528 10 | | f1476 11 | | f1460 11 |
| s 83 | -1.00 | TORS | 19 | 17 | 1 | 6 | HCCC | | -118.21 | | f1388 59 | |  | |  |
|  | 1.00 |  | 18 | 17 | 1 | 6 | HCCC | | 1.06 | |  | |  | |  |
|  | -1.00 |  | 28 | 22 | 26 | 25 | HCCC | | 60.21 | |  | |  | |  |
|  | 1.00 |  | 27 | 22 | 26 | 25 | HCCC | | -181.24 | |  | |  | |  |
| s 84 | 1.00 | TORS | 27 | 22 | 26 | 25 | HCCC | | -181.24 | | f312 23 | |  | |  |
|  | 1.00 |  | 28 | 22 | 26 | 25 | HCCC | | 60.21 | |  | |  | |  |
| s 85 | 1.00 | TORS | 29 | 25 | 21 | 33 | HCCN | | -142.91 | | f1286 13 | | f581 20 | |  |
| s 86 | 1.00 | TORS | 30 | 25 | 21 | 33 | HCCN | | -255.42 | | f1358 24 | | f1286 11 | |  |
| s 87 | 1.00 | TORS | 28 | 22 | 26 | 25 | HCCC | | 60.21 | | f1380 42 | | f1368 14 | |  |
|  | 1.00 |  | 31 | 26 | 25 | 21 | HCCC | | -191.97 | |  | |  | |  |
|  | -1.00 |  | 32 | 26 | 25 | 21 | HCCC | | -74.53 | |  | |  | |  |
|  | -1.00 |  | 27 | 22 | 26 | 25 | HCCC | | -181.24 | |  | |  | |  |
| s 88 | 1.00 | TORS | 28 | 22 | 26 | 25 | HCCC | | 60.21 | | f1387 55 | |  | |  |
|  | 1.00 |  | 18 | 17 | 1 | 6 | HCCC | | 1.06 | |  | |  | |  |
|  | -1.00 |  | 27 | 22 | 26 | 25 | HCCC | | -181.24 | |  | |  | |  |
|  | -1.00 |  | 19 | 17 | 1 | 6 | HCCC | | -118.21 | |  | |  | |  |
|  | 1.00 |  | 32 | 26 | 25 | 21 | HCCC | | -74.53 | |  | |  | |  |
| s 89 | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | 0.22 | | f109 34 | | f97 17 | |  |
| s 90 | -1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | -0.25 | | f455 62 | |  | |  |
|  | 1.00 |  | 1 | 2 | 3 | 4 | CCCC | | 0.16 | |  | |  | |  |
|  | -1.00 | OUT | 34 | 3 | 5 | 4 | OCCC | | 0.11 | |  | |  | |  |
|  | -1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | 0.22 | |  | |  | |  |
| s 91 | -1.00 | OUT | 13 | 1 | 5 | 6 | CCCC | | 0.54 | | f634 25 | | f561 14 | | f376 13 |
|  | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | 0.16 | |  | |  | |  |
|  | 1.00 |  | 2 | 3 | 4 | 5 | CCCC | | 0.22 | |  | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.25 | |  | |  | |  |
|  | -1.00 | OUT | 34 | 3 | 5 | 4 | OCCC | | 0.11 | |  | |  | |  |
| s 92 | 1.00 | TORS | 1 | 17 | 33 | 21 | CCNC | | -247.67 | | f35 77 | |  | |  |
|  | -1.00 |  | 6 | 1 | 17 | 33 | CCCN | | -237.30 | |  | |  | |  |
| s 93 | 1.00 | TORS | 22 | 20 | 33 | 17 | CCNC | | -193.21 | | f129 23 | | f44 17 | |  |
| s 94 | 1.00 | TORS | 17 | 33 | 21 | 25 | CNCC | | -182.85 | | f109 12 | | f97 32 | |  |
| s 95 | 1.00 | TORS | 26 | 22 | 20 | 33 | CCCN | | 48.08 | | f1116 11 | | f312 21 | |  |
| s 96 | 1.00 | TORS | 1 | 17 | 33 | 21 | CCNC | | -247.67 | | f19 79 | |  | |  |
|  | 1.00 |  | 6 | 1 | 17 | 33 | CCCN | | -237.30 | |  | |  | |  |
| s 97 | 1.00 | OUT | 36 | 25 | 33 | 21 | OCNC | | 1.54 | | f665 13 | | f634 13 | | f581 25 |
| s 98 | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | 0.16 | | f847 13 | | f717 18 | | f109 13 |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.25 | |  | |  | |  |
|  | 1.00 | OUT | 34 | 3 | 5 | 4 | OCCC | | 0.11 | |  | |  | |  |
|  | 1.00 |  | 13 | 1 | 5 | 6 | CCCC | | 0.54 | |  | |  | |  |
|  | -1.00 |  | 9 | 2 | 4 | 3 | CCCC | | 0.33 | |  | |  | |  |
| s 99 | -1.00 | OUT | 9 | 2 | 4 | 3 | CCCC | | 0.33 | | f176 50 | | f124 11 | |  |
|  | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | -0.25 | |  | |  | |  |
|  | -1.00 |  | 1 | 2 | 3 | 4 | CCCC | | 0.16 | |  | |  | |  |
|  | 1.00 | OUT | 13 | 1 | 5 | 6 | CCCC | | 0.54 | |  | |  | |  |
| s 100 | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | -0.25 | | f251 46 | |  | |  |
|  | 1.00 | OUT | 13 | 1 | 5 | 6 | CCCC | | 0.54 | |  | |  | |  |
|  | 1.00 |  | 9 | 2 | 4 | 3 | CCCC | | 0.33 | |  | |  | |  |
| s 101 | 1.00 | OUT | 20 | 17 | 21 | 33 | CCCN | | 5.83 | | f263 16 | |  | |  |
|  | 1.00 | TORS | 17 | 33 | 21 | 25 | CNCC | | -182.85 | |  | |  | |  |
| s 102 | 2 1.00 | OUT | 17 | 6 | 2 | 1 | CCCC | | 1.11 | | f376 10 | | f44 19 | |  |

Experimental and calculated wavenumbers of FT-IR spectra of compound 5 by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | IR calculated, scaled ν(cm-1) | IR calculated, unscaled ν(cm-1 | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % |
| 3418 | 3680,097 | 3828,25 | s1 | 100 |  |  |  |  |  |  |
| 3034 | 3021,414 | 3143,05 | s2 | 97 |  |  |  |  |  |  |
| 3024 | 3013,887 | 3135,22 | s3 | 96 |  |  |  |  |  |  |
| 2995 | 2996,257 | 3116,88 | s16 | -96 |  |  |  |  |  |  |
| - | 2984,75 | 3104,91 | s7 | -98 |  |  |  |  |  |  |
| - | 2981,501 | 3101,53 | s12 | 85 | s14 | -10 |  |  |  |  |
| - | 2981,318 | 3101,34 | s5 | -22 | s6 | 78 |  |  |  |  |
| 2958 | 2959,352 | 3078,49 | s8 | -98 |  |  |  |  |  |  |
| - | 2954,757 | 3073,71 | s17 | 88 |  |  |  |  |  |  |
| - | 2952,383 | 3071,24 | s4 | -100 |  |  |  |  |  |  |
| - | 2943,058 | 3061,54 | s20 | -74 |  |  |  |  |  |  |
| 2935 | 2938,358 | 3056,65 | s18 | 77 | s21 | -12 |  |  |  |  |
| 2928 | 2928,004 | 3045,88 | s14 | 77 |  |  |  |  |  |  |
| - | 2920,545 | 3038,12 | s15 | 69 |  |  |  |  |  |  |
| - | 2913,739 | 3031,04 | s10 | 80 | s11 | -12 |  |  |  |  |
| - | 2909,423 | 3026,55 | s5 | 77 | s6 | 21 |  |  |  |  |
| - | 2909,076 | 3026,19 | s21 | 74 |  |  |  |  |  |  |
| - | 2908,452 | 3025,54 | s9 | 89 |  |  |  |  |  |  |
| - | 2901,905 | 3018,73 | s15 | -11 | s19 | 84 |  |  |  |  |
| 2899 | 2890,812 | 3007,19 | s13 | 80 |  |  |  |  |  |  |
| 2852 | 2877,056 | 2992,88 | s10 | 10 | s11 | 81 |  |  |  |  |
| 1633 | 1676,565 | 1744,06 | s22 | 87 |  |  |  |  |  |  |
| 1612 | 1592,74 | 1656,86 | s23 | 59 | s43 | 14 |  |  |  |  |
| 1512 | 1558,181 | 1620,91 | s26 | 54 |  |  |  |  |  |  |
| 1496 | 1483,661 | 1543,39 | s42 | -35 | s69 | -12 |  |  |  |  |
| 1464 | 1451,332 | 1509,76 | s61 | 56 |  |  |  |  |  |  |
| 1458 | 1447,41 | 1505,68 | s49 | 62 | s79 | 21 |  |  |  |  |
| 1454 | 1441,825 | 1499,87 | s53 | 71 |  |  |  |  |  |  |
| 1444 | 1437,134 | 1494,99 | s50 | 73 |  |  |  |  |  |  |
| 1438 | 1434,173 | 1491,91 | s46 | 64 | s83 | 20 |  |  |  |  |
| 1431 | 1431,751 | 1489,39 | s57 | 79 |  |  |  |  |  |  |
| 1417 | 1425,618 | 1483,01 | s59 | 72 |  |  |  |  |  |  |
| 1419 | 1423,589 | 1480,9 | s55 | 72 |  |  |  |  |  |  |
| - | 1422,186 | 1479,44 | s44 | -74 | s81 | 23 |  |  |  |  |
| - | 1419,83 | 1476,99 | s47 | 65 | s82 | 10 |  |  |  |  |
| 1380 | 1385,666 | 1441,45 | s28 | 38 |  |  |  |  |  |  |
| 1367 | 1366,853 | 1421,88 | s48 | 73 |  |  |  |  |  |  |
| 1363 | 1363,989 | 1418,9 | s45 | 87 |  |  |  |  |  |  |
| 1353 | 1353,424 | 1407,91 | s48 | 16 |  |  |  |  |  |  |
| 1340 | 1332,391 | 1386,03 | s52 | 34 | s88 | -28 |  |  |  |  |
| 1338 | 1329,007 | 1382,51 | s52 | -11 | s94 | -26 |  |  |  |  |
| 1325 | 1323,989 | 1377,29 | s58 | -17 | s93 | -10 | s95 | 10 | s96 | -21 |
| 1321 | 1318,5 | 1371,58 | s93 | -43 |  |  |  |  |  |  |
| 1302 | 1293,218 | 1345,28 | s25 | -35 | s51 | 19 |  |  |  |  |
| 1293 | 1287,171 | 1338,99 | s41 | 14 | s43 | -19 |  |  |  |  |
| - | 1283,009 | 1334,66 | s60 | 37 | s96 | -12 |  |  |  |  |
| 1278 | 1269,656 | 1320,77 | s43 | 19 | s56 | -13 |  |  |  |  |
| 1261 | 1255,035 | 1305,56 | s27 | -46 |  |  |  |  |  |  |
| 1246 | 1230,637 | 1280,18 | s54 | -41 | s90 | 18 |  |  |  |  |
| 1232 | 1223,418 | 1272,67 | s43 | -11 | s51 | -12 |  |  |  |  |
| 1201 | 1209,546 | 1258,24 | s54 | 13 | s58 | 13 | s90 | 15 |  |  |
| 1193 | 1201,788 | 1250,17 | s30 | 13 | s41 | -15 | s65 | -15 |  |  |
| 1184 | 1196,203 | 1244,36 | s85 | 11 |  |  |  |  |  |  |
| 1153 | 1171,988 | 1219,17 | s32 | -11 | s42 | -48 |  |  |  |  |
| 1145 | 1165,567 | 1212,49 | s92 | 52 |  |  |  |  |  |  |
| - | 1135,132 | 1180,83 | s41 | -11 |  |  |  |  |  |  |
| - | 1126,346 | 1171,69 | s41 | 25 |  |  |  |  |  |  |
| 1082 | 1084,202 | 1127,85 | s104 | -10 | s106 | 12 |  |  |  |  |
| - | 1066,005 | 1108,92 | s29 | -11 | s34 | 14 | s56 | 23 |  |  |
| 1045 | 1049,826 | 1092,09 | s24 | 18 |  |  |  |  |  |  |
| - | 1028,927 | 1070,35 | s37 | -51 |  |  |  |  |  |  |
| 1012 | 1024,909 | 1066,17 | s44 | -15 | s81 | 47 | s82 | 12 |  |  |
| - | 1019,516 | 1060,56 | s47 | 13 | s81 | -18 | s82 | 39 |  |  |
| 991 | 1000,463 | 1040,74 | s46 | -14 | s83 | -49 |  |  |  |  |
| 979 | 977,6613 | 1017,02 | s36 | 13 | s40 | 11 |  |  |  |  |
| 977 | 974,6621 | 1013,9 | s49 | 12 | s79 | 40 |  |  |  |  |
| 974 | 968,0483 | 1007,02 | s36 | 11 |  |  |  |  |  |  |
| 960 | 934,7777 | 972,41 | s38 | -13 |  |  |  |  |  |  |
| 943 | 923,9054 | 961,1 |  |  |  |  |  |  |  |  |
| - | 921,0023 | 958,08 | s36 | 10 |  |  |  |  |  |  |
| 881 | 878,3783 | 913,74 | s77 | -73 |  |  |  |  |  |  |
| 846 | 835,8792 | 869,53 | s75 | 19 | s94 | 10 |  |  |  |  |
| - | 825,1319 | 858,35 | s74 | 11 |  |  |  |  |  |  |
| 837 | 823,6995 | 856,86 | s78 | 69 |  |  |  |  |  |  |
| - | 801,8876 | 834,17 | s24 | -17 | s30 | -14 | s32 | 16 | s69 | 14 |
| 815 | 798,1674 | 830,3 |  |  |  |  |  |  |  |  |
| 750 | 740,2971 | 770,1 | s29 | 11 | s38 | -14 |  |  |  |  |
| 736 | 735,8752 | 765,5 | s31 | 11 | s38 | 17 |  |  |  |  |
| 702 | 721,7152 | 750,77 | s31 | 16 | s67 | -12 |  |  |  |  |
| 682 | 692,857 | 720,75 |  |  |  |  |  |  |  |  |
| - | 687,7621 | 715,45 | s29 | -10 | s91 | 10 |  |  |  |  |
| - | 684,4937 | 712,05 | s65 | -13 |  |  |  |  |  |  |
| - | 623,4223 | 648,52 | s107 | -17 |  |  |  |  |  |  |
| - | 577,7798 | 601,04 | s62 | -29 |  |  |  |  |  |  |
| - | 559,3997 | 581,92 | s67 | 19 |  |  |  |  |  |  |
| - | 518,0926 | 538,95 | s66 | 45 |  |  |  |  |  |  |
| - | 490,263 | 510 | s74 | 17 |  |  |  |  |  |  |
| - | 454,445 | 472,74 | s72 | -15 | s101 | -39 |  |  |  |  |
| - | 443,1401 | 460,98 | s72 | 40 |  |  |  |  |  |  |
| - | 441,6404 | 459,42 | s30 | 10 | s63 | 40 |  |  |  |  |
| - | 394,8636 | 410,76 | s40 | 22 |  |  |  |  |  |  |
| - | 367,0243 | 381,8 | s107 | -12 | s109 | -10 |  |  |  |  |
| - | 353,8353 | 368,08 | s68 | 14 |  |  |  |  |  |  |
| - | 326,0922 | 339,22 | s75 | 17 | s110 | 14 |  |  |  |  |
| - | 316,0081 | 328,73 | s76 | 69 |  |  |  |  |  |  |
| - | 304,2611 | 316,51 | s39 | 14 | s68 | -23 | s76 | 14 |  |  |
| - | 299,7333 | 311,8 | s64 | 51 |  |  |  |  |  |  |
| - | 278,8731 | 290,1 | s39 | 58 |  |  |  |  |  |  |
| - | 271,5096 | 282,44 | s109 | 14 |  |  |  |  |  |  |
| - | 248,3038 | 258,3 | s99 | -24 | s108 | 11 |  |  |  |  |
| - | 234,5668 | 244,01 | s70 | -36 |  |  |  |  |  |  |
| - | 176,735 | 183,85 | s109 | -10 |  |  |  |  |  |  |
| - | 152,5102 | 158,65 | s102 | -13 | s104 | -15 |  |  |  |  |
| - | 139,6481 | 145,27 | s84 | 17 | s104 | 17 |  |  |  |  |
| - | 123,2867 | 128,25 | s84 | 35 |  |  |  |  |  |  |
| - | 112,251 | 116,77 | s80 | 87 |  |  |  |  |  |  |
| - | 107,6271 | 111,96 | s103 | 44 |  |  |  |  |  |  |
| - | 98,53325 | 102,5 | s84 | 10 | s98 | 42 |  |  |  |  |
| - | 55,84192 | 58,09 | s71 | -22 | s97 | -28 |  |  |  |  |
| - | 43,07585 | 44,81 | s111 | -58 |  |  |  |  |  |  |
| - | 18,32238 | 19,06 | \* | 20,65 | s100 | -79 |  |  |  |  |

Scaling factor = 0.9613, (-)PED% - asymmetric vibrations

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| s 1 | 1.00 | STRE | 36 | 37 | OH | 0.963803 | | f3828 100 | |  | |  | |
| s 2 | 1.00 | STRE | 2 | 7 | CH | 1.086094 | | f3143 97 | |  | |  | |
| s 3 | 1.00 | STRE | 5 | 8 | CH | 1.086773 | | f3135 96 | |  | |  | |
| s 4 | 1.00 | STRE | 9 | 10 | CH | 1.093176 | | f3071 100 | |  | |  | |
|  | -1.00 |  | 9 | 11 | CH | 1.093221 | |  | |  | |  | |
| s 5 | 1.00 | STRE | 9 | 10 | CH | 1.093176 | | f3101 22 | | f3027 77 | |  | |
|  | 1.00 |  | 9 | 11 | CH | 1.093221 | |  | |  | |  | |
| s 6 | 1.00 | STRE | 9 | 12 | CH | 1.090816 | | f3101 78 | | f3027 21 | |  | |
| s 7 | 1.00 | STRE | 13 | 14 | CH | 1.090903 | | f3105 98 | |  | |  | |
|  | -1.00 |  | 13 | 16 | CH | 1.091237 | |  | |  | |  | |
| s 8 | -1.00 | STRE | 13 | 14 | CH | 1.090903 | | f3079 98 | |  | |  | |
|  | 1.00 |  | 13 | 15 | CH | 1.094168 | |  | |  | |  | |
|  | -1.00 |  | 13 | 16 | CH | 1.091237 | |  | |  | |  | |
| s 9 | 1.00 | STRE | 13 | 14 | CH | 1.090903 | | f3026 89 | |  | |  | |
|  | 1.00 |  | 13 | 15 | CH | 1.094168 | |  | |  | |  | |
|  | 1.00 |  | 13 | 16 | CH | 1.091237 | |  | |  | |  | |
| s 10 | 1.00 | STRE | 17 | 18 | CH | 1.094768 | | f3031 80 | | f2993 10 | |  | |
| s 11 | 1.00 | STRE | 17 | 19 | CH | 1.096479 | | f3031 12 | | f2993 81 | |  | |
| s 12 | 1.00 | STRE | 20 | 23 | CH | 1.089883 | | f3102 85 | |  | |  | |
| s 13 | 1.00 | STRE | 22 | 27 | CH | 1.096052 | | f3007 80 | |  | |  | |
|  | 1.00 |  | 22 | 28 | CH | 1.095442 | |  | |  | |  | |
| s 14 | 1.00 | STRE | 20 | 24 | CH | 1.093007 | | f3102 10 | | f3046 77 | |  | |
|  | 1.00 |  | 22 | 28 | CH | 1.095442 | |  | |  | |  | |
| s 15 | 1.00 | STRE | 22 | 28 | CH | 1.095442 | | f3038 69 | | f3019 11 | |  | |
| s 16 | 1.00 | STRE | 25 | 30 | CH | 1.089132 | | f3117 96 | |  | |  | |
|  | -1.00 |  | 25 | 31 | CH | 1.090253 | |  | |  | |  | |
| s 17 | 1.00 | STRE | 25 | 30 | CH | 1.089132 | | f3074 88 | |  | |  | |
|  | 1.00 |  | 25 | 31 | CH | 1.090253 | |  | |  | |  | |
| s 18 | 1.00 | STRE | 26 | 32 | CH | 1.094916 | | f3057 77 | |  | |  | |
|  | -1.00 |  | 26 | 33 | CH | 1.093822 | |  | |  | |  | |
| s 19 | 1.00 | STRE | 26 | 32 | CH | 1.094916 | | f3019 84 | |  | |  | |
|  | 1.00 |  | 26 | 33 | CH | 1.093822 | |  | |  | |  | |
| s 20 | 1.00 | STRE | 29 | 34 | CH | 1.092489 | | f3062 74 | |  | |  | |
|  | -1.00 |  | 29 | 35 | CH | 1.093586 | |  | |  | |  | |
| s 21 | 1.00 | STRE | 29 | 35 | CH | 1.093586 | | f3057 12 | | f3026 74 | |  | |
|  | 1.00 |  | 29 | 34 | CH | 1.092489 | |  | |  | |  | |
| s 22 | 1.00 | STRE | 38 | 21 | OC | 1.213127 | | f1744 87 | |  | |  | |
| s 23 | 1.00 | STRE | 4 | 5 | CC | 1.390946 | | f1657 59 | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.395784 | |  | |  | |  | |
|  | -1.00 |  | 2 | 3 | CC | 1.391826 | |  | |  | |  | |
|  | -1.00 |  | 5 | 6 | CC | 1.393583 | |  | |  | |  | |
| s 24 | 1.00 | STRE | 36 | 4 | OC | 1.372291 | | f1092 18 | | f834 17 | |  | |
| s 25 | -1.00 | STRE | 5 | 6 | CC | 1.393583 | | f1345 35 | |  | |  | |
|  | -1.00 |  | 3 | 4 | CC | 1.395748 | |  | |  | |  | |
|  | 1.00 |  | 2 | 3 | CC | 1.391826 | |  | |  | |  | |
|  | 1.00 |  | 4 | 5 | CC | 1.390946 | |  | |  | |  | |
| s 26 | 1.00 | STRE | 3 | 4 | CC | 1.395748 | | f1621 48 | |  | |  | |
|  | -1.00 |  | 5 | 6 | CC | 1.393583 | |  | |  | |  | |
| s 27 | -1.00 | STRE | 36 | 4 | OC | 1.372291 | | f1306 46 | |  | |  | |
|  | -1.00 |  | 6 | 13 | CC | 1.507585 | |  | |  | |  | |
|  | 1.00 |  | 4 | 5 | CC | 1.390946 | |  | |  | |  | |
|  | 1.00 |  | 2 | 3 | CC | 1.391826 | |  | |  | |  | |
| s 28 | -1.00 | STRE | 1 | 2 | CC | 1.395784 | | f1441 38 | |  | |  | |
|  | 1.00 |  | 4 | 5 | CC | 1.390946 | |  | |  | |  | |
|  | -1.00 |  | 36 | 4 | OC | 1.372291 | |  | |  | |  | |
|  | 1.00 |  | 5 | 6 | CC | 1.393583 | |  | |  | |  | |
| s 29 | 1.00 | STRE | 39 | 21 | NC | 1.412523 | | f1109 11 | | f770 12 | | f715 10 | |
| s 30 | 1.00 | STRE | 9 | 3 | CC | 1.504418 | | f1250 13 | | f834 14 | | f460 10 | |
| s 31 | 1.00 | STRE | 6 | 13 | CC | 1.507585 | | f766 11 | | f751 15 | |  | |
|  | 1.00 |  | 3 | 4 | CC | 1.395748 | |  | |  | |  | |
|  | 1.00 |  | 5 | 6 | CC | 1.393583 | |  | |  | |  | |
|  | 1.00 |  | 2 | 3 | CC | 1.391826 | |  | |  | |  | |
| s 32 | 1.00 | STRE | 17 | 1 | CC | 1.514998 | | f1219 11 | | f834 16 | |  | |
| s 33 | 1.00 | STRE | 25 | 21 | CC | 1.514701 | | f770 10 | |  | |  | |
| s 34 | 1.00 | STRE | 39 | 17 | NC | 1.469614 | | f1109 14 | |  | |  | |
| s 35 | 1.00 | STRE | 39 | 20 | NC | 1.473417 | |  | |  | |  | |
| s 36 | 1.00 | STRE | 22 | 20 | CC | 1.539433 | | f1017 13 | | f1007 11 | | f958 11 | |
| s 37 | -1.00 | STRE | 26 | 29 | CC | 1.547876 | | f1070 50 | |  | |  | |
|  | 1.00 |  | 22 | 26 | CC | 1.545572 | |  | |  | |  | |
| s 38 | 1.00 | STRE | 22 | 26 | CC | 1.545572 | | f972 12 | | f770 14 | | f766 17 | |
|  | 1.00 |  | 26 | 29 | CC | 1.547876 | |  | |  | |  | |
| s 39 | 1.00 | BEND | 3 | 4 | 5 | CCC | 120.83 | | f317 12 | | f290 53 | |  | |  |
|  | 1.00 |  | 2 | 3 | 9 | CCC | 122.44 | |  | |  | |  | |  |
|  | 1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | 1.00 |  | 5 | 4 | 36 | CCO | 121.94 | |  | |  | |  | |  |
| s 40 | 1.00 | BEND | 29 | 26 | 22 | CCC | 116.21 | | f1017 11 | | f510 10 | | f411 23 | |  |
| s 41 | 1.00 | BEND | 37 | 36 | 4 | HOC | 109.46 | | f1339 15 | | f1250 14 | | f1181 12 | | f1172 25 |
| s 42 | 1.00 | BEND | 7 | 2 | 3 | HCC | 117.82 | | f1543 35 | | f1219 48 | |  | |  |
|  | -1.00 |  | 8 | 5 | 6 | HCC | 119.12 | |  | |  | |  | |  |
| s 43 | 1.00 | BEND | 7 | 2 | 3 | HCC | 117.82 | | f1657 14 | | f1339 19 | | f1321 19 | | f1273 12 |
|  | 1.00 |  | 8 | 5 | 6 | HCC | 119.12 | |  | |  | |  | |  |
| s 44 | 1.00 | BEND | 10 | 9 | 12 | HCH | 108.31 | | f1479 74 | | f1066 15 | |  | |  |
|  | -1.00 |  | 11 | 9 | 12 | HCH | 108.32 | |  | |  | |  | |  |
| s 45 | 1.00 | BEND | 10 | 9 | 11 | HCH | 106.59 | | f1419 88 | |  | |  | |  |
|  | 1.00 |  | 10 | 9 | 12 | HCH | 108.31 | |  | |  | |  | |  |
|  | 1.00 |  | 11 | 9 | 12 | HCH | 108.32 | |  | |  | |  | |  |
| s 46 | 1.00 | BEND | 14 | 13 | 15 | HCH | 107.68 | | f1492 64 | | f1041 14 | |  | |  |
|  | -1.00 |  | 10 | 9 | 11 | HCH | 106.59 | |  | |  | |  | |  |
|  | -1.00 |  | 15 | 13 | 16 | HCH | 106.78 | |  | |  | |  | |  |
|  | 1.00 |  | 11 | 9 | 12 | HCH | 108.32 | |  | |  | |  | |  |
| s 47 | 1.00 | BEND | 14 | 13 | 16 | HCH | 108.71 | | f1477 65 | | f1061 14 | |  | |  |
|  | -1.00 |  | 14 | 13 | 15 | HCH | 107.68 | |  | |  | |  | |  |
| s 48 | 1.00 | BEND | 15 | 13 | 16 | HCH | 106.78 | | f1422 73 | | f1408 17 | |  | |  |
|  | 1.00 |  | 14 | 13 | 16 | HCH | 108.71 | |  | |  | |  | |  |
|  | 1.00 |  | 14 | 13 | 15 | HCH | 107.68 | |  | |  | |  | |  |
| s 49 | -1.00 | BEND | 10 | 9 | 11 | HCH | 106.59 | | f1506 62 | | f1014 12 | |  | |  |
|  | -1.00 |  | 14 | 13 | 15 | HCH | 107.68 | |  | |  | |  | |  |
|  | 1.00 |  | 15 | 13 | 16 | HCH | 106.78 | |  | |  | |  | |  |
|  | 1.00 |  | 11 | 9 | 12 | HCH | 108.32 | |  | |  | |  | |  |
| s 50 | 1.00 | BEND | 32 | 26 | 33 | HCH | 105.98 | | f1495 73 | |  | |  | |  |
|  | 1.00 |  | 23 | 20 | 24 | HCH | 107.45 | |  | |  | |  | |  |
|  | 1.00 |  | 27 | 22 | 28 | HCH | 105.93 | |  | |  | |  | |  |
|  | -1.00 |  | 18 | 17 | 19 | HCH | 105.83 | |  | |  | |  | |  |
| s 51 | 1.00 | BEND | 19 | 17 | 1 | HCC | 108.72 | | f1345 18 | | f1273 12 | |  | |  |
| s 52 | 1.00 | BEND | 23 | 20 | 22 | HCC | 110.38 | | f1386 30 | | f1383 16 | |  | |  |
|  | -1.00 |  | 27 | 22 | 26 | HCC | 108.72 | |  | |  | |  | |  |
| s 53 | -1.00 | BEND | 34 | 29 | 35 | HCH | 105.78 | | f1500 71 | |  | |  | |  |
|  | 1.00 |  | 23 | 20 | 24 | HCH | 107.45 | |  | |  | |  | |  |
| s 54 | 1.00 | BEND | 30 | 25 | 29 | HCC | 110.89 | | f1280 40 | | f1258 13 | |  | |  |
|  | 1.00 |  | 27 | 22 | 26 | HCC | 108.72 | |  | |  | |  | |  |
| s 55 | 1.00 | BEND | 27 | 22 | 28 | HCH | 105.93 | | f1481 72 | |  | |  | |  |
|  | 1.00 |  | 30 | 25 | 31 | HCH | 107.79 | |  | |  | |  | |  |
|  | -1.00 |  | 34 | 29 | 35 | HCH | 105.78 | |  | |  | |  | |  |
| s 56 | -1.00 | BEND | 23 | 20 | 22 | HCC | 110.38 | | f1321 15 | | f1109 25 | |  | |  |
|  | -1.00 |  | 27 | 22 | 26 | HCC | 108.72 | |  | |  | |  | |  |
|  | 1.00 |  | 30 | 25 | 29 | HCC | 110.89 | |  | |  | |  | |  |
| s 57 | -1.00 | BEND | 23 | 20 | 24 | HCH | 107.45 | | f1489 79 | |  | |  | |  |
|  | 1.00 |  | 30 | 25 | 31 | HCH | 107.79 | |  | |  | |  | |  |
|  | 1.00 |  | 32 | 26 | 33 | HCH | 105.98 | |  | |  | |  | |  |
|  | -1.00 |  | 34 | 29 | 35 | HCH | 105.78 | |  | |  | |  | |  |
| s 58 | 1.00 | BEND | 32 | 26 | 29 | HCC | 109.86 | | f1377 18 | | f1258 13 | |  | |  |
| s 59 | 1.00 | BEND | 23 | 20 | 24 | HCH | 107.45 | | f1483 72 | |  | |  | |  |
|  | -1.00 |  | 27 | 22 | 28 | HCH | 105.93 | |  | |  | |  | |  |
|  | 1.00 |  | 30 | 25 | 31 | HCH | 107.79 | |  | |  | |  | |  |
|  | -1.00 |  | 32 | 26 | 33 | HCH | 105.98 | |  | |  | |  | |  |
| s 60 | 1.00 | BEND | 30 | 25 | 29 | HCC | 110.89 | | f1335 37 | |  | |  | |  |
|  | 1.00 |  | 34 | 29 | 26 | HCC | 108.25 | |  | |  | |  | |  |
| s 61 | 1.00 | BEND | 18 | 17 | 19 | HCH | 105.83 | | f1510 56 | |  | |  | |  |
|  | 1.00 |  | 23 | 20 | 24 | HCH | 107.45 | |  | |  | |  | |  |
|  | 1.00 |  | 30 | 25 | 31 | HCH | 107.79 | |  | |  | |  | |  |
| s 62 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | | f649 11 | | f601 28 | |  | |  |
|  | -1.00 |  | 2 | 1 | 17 | CCC | 119.22 | |  | |  | |  | |  |
|  | 1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | 1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | CNC | 120.51 | |  | |  | |  | |  |
|  | -1.00 |  | 25 | 21 | 38 | CCO | 121.27 | |  | |  | |  | |  |
|  | -1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 63 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | | f460 28 | |  | |  | |  |
|  | -1.00 |  | 2 | 1 | 17 | CCC | 119.22 | |  | |  | |  | |  |
|  | 1.00 |  | 2 | 3 | 9 | CCC | 122.44 | |  | |  | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | CCC | 120.83 | |  | |  | |  | |  |
|  | 1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 4 | 36 | CCO | 121.94 | |  | |  | |  | |  |
|  | 1.00 |  | 5 | 6 | 13 | CCC | 119.40 | |  | |  | |  | |  |
|  | -1.00 |  | 17 | 39 | 21 | CNC | 120.51 | |  | |  | |  | |  |
|  | 1.00 |  | 25 | 21 | 38 | CCO | 121.27 | |  | |  | |  | |  |
|  | -1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 64 | 1.00 | BEND | 5 | 6 | 13 | CCC | 119.40 | | f312 47 | |  | |  | |  |
| s 65 | 1.00 | BEND | 2 | 1 | 17 | CCC | 119.22 | | f1250 17 | | f712 14 | |  | |  |
|  | -1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | -1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 6 | 13 | CCC | 119.40 | |  | |  | |  | |  |
| s 66 | 1.00 | BEND | 2 | 1 | 17 | CCC | 119.22 | | f1621 11 | | f539 35 | |  | |  |
|  | 1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | 1.00 |  | 5 | 4 | 36 | CCO | 121.94 | |  | |  | |  | |  |
| s 67 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | | f751 14 | | f582 22 | |  | |  |
|  | -1.00 |  | 2 | 1 | 17 | CCC | 119.22 | |  | |  | |  | |  |
|  | 1.00 |  | 2 | 3 | 9 | CCC | 122.44 | |  | |  | |  | |  |
|  | -1.00 |  | 3 | 4 | 5 | CCC | 120.83 | |  | |  | |  | |  |
|  | 1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | 1.00 |  | 5 | 6 | 13 | CCC | 119.40 | |  | |  | |  | |  |
|  | 1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 68 | -1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | | f368 12 | | f317 27 | |  | |  |
|  | 1.00 |  | 2 | 1 | 17 | CCC | 119.22 | |  | |  | |  | |  |
|  | -1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 4 | 36 | CCO | 121.94 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 6 | 13 | CCC | 119.40 | |  | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | CNC | 120.51 | |  | |  | |  | |  |
|  | 1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 69 | 1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | | f1543 12 | | f834 15 | |  | |  |
|  | 1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | CCC | 120.83 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 4 | 36 | CCO | 121.94 | |  | |  | |  | |  |
|  | 1.00 |  | 20 | 39 | 21 | CNC | 110.47 | |  | |  | |  | |  |
| s 70 | -1.00 | BEND | 2 | 1 | 17 | CCC | 119.22 | | f244 35 | |  | |  | |  |
|  | -1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | -1.00 |  | 2 | 3 | 9 | CCC | 122.44 | |  | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | CNC | 120.51 | |  | |  | |  | |  |
|  | 1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 71 | 1.00 | BEND | 39 | 17 | 1 | NCC | 113.78 | | f58 18 | |  | |  | |  |
| s 72 | 1.00 | BEND | 17 | 39 | 21 | CNC | 120.51 | | f473 15 | | f461 32 | |  | |  |
|  | 1.00 |  | 25 | 21 | 38 | CCO | 121.27 | |  | |  | |  | |  |
| s 73 | -1.00 | BEND | 1 | 2 | 3 | CCC | 123.58 | |  | |  | |  | |  |
|  | 1.00 |  | 2 | 1 | 17 | CCC | 119.22 | |  | |  | |  | |  |
|  | -1.00 |  | 2 | 3 | 4 | CCC | 116.77 | |  | |  | |  | |  |
|  | -1.00 |  | 4 | 5 | 6 | CCC | 121.84 | |  | |  | |  | |  |
|  | -1.00 |  | 5 | 6 | 13 | CCC | 119.40 | |  | |  | |  | |  |
|  | 1.00 |  | 20 | 39 | 21 | CNC | 110.47 | |  | |  | |  | |  |
|  | -1.00 |  | 25 | 21 | 39 | CCN | 117.46 | |  | |  | |  | |  |
| s 74 | 1.00 | BEND | 22 | 20 | 39 | CCN | 112.71 | | f858 11 | | f510 19 | |  | |  |
| s 75 | 1.00 | BEND | 26 | 22 | 20 | CCC | 115.58 | | f870 20 | | f339 17 | |  | |  |
| s 76 | 1.00 | TORS | 37 | 36 | 4 | 5 | HOCC | | -1.18 | | f329 68 | | f317 14 | |  |
| s 77 | 1.00 | TORS | 7 | 2 | 3 | 9 | HCCC | | 0.47 | | f914 72 | |  | |  |
| s 78 | 1.00 | TORS | 8 | 5 | 6 | 13 | HCCC | | -0.81 | | f857 71 | |  | |  |
| s 79 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.91 | | f1506 22 | | f1014 40 | |  |
|  | -1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.88 | |  | |  | |  |
|  | -1.00 |  | 15 | 13 | 6 | 5 | HCCC | | -126.56 | |  | |  | |  |
|  | 1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -245.61 | |  | |  | |  |
| s 80 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.91 | | f117 87 | |  | |  |
|  | 1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.88 | |  | |  | |  |
|  | 1.00 |  | 12 | 9 | 3 | 4 | HCCC | | -180.49 | |  | |  | |  |
| s 81 | -1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.91 | | f1479 23 | | f1066 47 | | f1061 19 |
|  | 1.00 |  | 12 | 9 | 3 | 4 | HCCC | | -180.49 | |  | |  | |  |
| s 82 | 1.00 | TORS | 14 | 13 | 6 | 5 | HCCC | | -6.73 | | f1477 10 | | f1066 13 | | f1061 40 |
| s 83 | 1.00 | TORS | 10 | 9 | 3 | 4 | HCCC | | 58.91 | | f1492 20 | | f1041 49 | |  |
|  | -1.00 |  | 11 | 9 | 3 | 4 | HCCC | | -59.88 | |  | |  | |  |
|  | 1.00 |  | 15 | 13 | 6 | 5 | HCCC | | -126.56 | |  | |  | |  |
|  | -1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -245.61 | |  | |  | |  |
| s 84 | 1.00 | TORS | 15 | 13 | 6 | 5 | HCCC | | -126.56 | | f145 17 | | f128 35 | |  |
|  | 1.00 |  | 16 | 13 | 6 | 5 | HCCC | | -245.61 | |  | |  | |  |
| s 85 | 1.00 | TORS | 18 | 17 | 1 | 6 | HCCC | | -57.46 | | f1510 10 | | f1408 10 | | f1244 11 |
| s 86 | 1.00 | TORS | 19 | 17 | 1 | 6 | HCCC | | -172.51 | | f961 10 | |  | |  |
| s 87 | 1.00 | TORS | 23 | 20 | 39 | 17 | HCNC | | -192.78 | |  | |  | |  |
| s 88 | 1.00 | TORS | 24 | 20 | 39 | 17 | HCNC | | 51.38 | | f1386 30 | |  | |  |
|  | -1.00 |  | 27 | 22 | 26 | 29 | HCCC | | -52.80 | |  | |  | |  |
|  | -1.00 |  | 33 | 26 | 29 | 25 | HCCC | | -197.82 | |  | |  | |  |
| s 89 | 1.00 | TORS | 27 | 22 | 26 | 29 | HCCC | | -52.80 | |  | |  | |  |
|  | 1.00 |  | 28 | 22 | 26 | 29 | HCCC | | -167.70 | |  | |  | |  |
|  | -1.00 |  | 32 | 26 | 29 | 25 | HCCC | | 47.48 | |  | |  | |  |
|  | -1.00 |  | 33 | 26 | 29 | 25 | HCCC | | -197.82 | |  | |  | |  |
| s 90 | 1.00 | TORS | 28 | 22 | 26 | 29 | HCCC | | -167.70 | | f1280 17 | | f1258 14 | |  |
|  | -1.00 |  | 31 | 25 | 21 | 39 | HCCN | | -62.27 | |  | |  | |  |
| s 91 | 1.00 | TORS | 30 | 25 | 21 | 39 | HCCN | | -180.14 | |  | |  | |  |
| s 92 | 1.00 | TORS | 28 | 22 | 26 | 29 | HCCC | | -167.70 | | f1213 53 | |  | |  |
|  | 1.00 |  | 31 | 25 | 21 | 39 | HCCN | | -62.27 | |  | |  | |  |
|  | 1.00 |  | 33 | 26 | 29 | 25 | HCCC | | -197.82 | |  | |  | |  |
| s 93 | -1.00 | TORS | 24 | 20 | 39 | 17 | HCNC | | 51.38 | | f1377 11 | | f1371 40 | |  |
|  | 1.00 |  | 28 | 22 | 26 | 29 | HCCC | | -167.70 | |  | |  | |  |
|  | 1.00 |  | 32 | 26 | 29 | 25 | HCCC | | 47.48 | |  | |  | |  |
|  | -1.00 |  | 33 | 26 | 29 | 25 | HCCC | | -197.82 | |  | |  | |  |
| s 94 | 1.00 | TORS | 24 | 20 | 39 | 17 | HCNC | | 51.38 | | f1383 24 | | f870 10 | |  |
|  | 1.00 |  | 27 | 22 | 26 | 29 | HCCC | | -52.80 | |  | |  | |  |
|  | -1.00 |  | 28 | 22 | 26 | 29 | HCCC | | -167.70 | |  | |  | |  |
|  | 1.00 |  | 32 | 26 | 29 | 25 | HCCC | | 47.48 | |  | |  | |  |
| s 95 | 1.00 | TORS | 34 | 29 | 26 | 22 | HCCC | | -199.07 | | f1377 10 | |  | |  |
| s 96 | 1.00 | TORS | 35 | 29 | 26 | 22 | HCCC | | 46.69 | | f1377 21 | | f1335 12 | |  |
| s 97 | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | 0.73 | | f58 32 | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
|  | -1.00 |  | 6 | 1 | 17 | 39 | CCCN | | 59.95 | |  | |  | |  |
|  | -1.00 |  | 17 | 39 | 20 | 22 | CNCC | | -71.07 | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | 25 | CNCC | | 35.03 | |  | |  | |  |
|  | 1.00 | OUT | 38 | 25 | 39 | 21 | OCNC | | 9.81 | |  | |  | |  |
| s 98 | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | 0.73 | | f103 41 | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
|  | -1.00 |  | 17 | 39 | 21 | 25 | CNCC | | 35.03 | |  | |  | |  |
| s 99 | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | -0.01 | | f715 11 | | f258 28 | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
| s 100 | 1.00 | TORS | 21 | 39 | 17 | 1 | CNCC | | 64.81 | | f21 78 | |  | |  |
| s 101 | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | -0.01 | | f473 15 | | f103 22 | |  |
|  | -1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | 25 | CNCC | | 35.03 | |  | |  | |  |
| s 102 | -1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | -0.01 | | f159 11 | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
|  | 1.00 |  | 6 | 1 | 17 | 39 | CCCN | | 59.95 | |  | |  | |  |
|  | -1.00 |  | 17 | 39 | 20 | 22 | CNCC | | -71.07 | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | 25 | CNCC | | 35.03 | |  | |  | |  |
|  | 1.00 | OUT | 38 | 25 | 39 | 21 | OCNC | | 9.81 | |  | |  | |  |
| s 103 | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | 0.73 | | f112 45 | |  | |  |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | -0.50 | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 20 | 22 | CNCC | | -71.07 | |  | |  | |  |
|  | 1.00 |  | 17 | 39 | 21 | 25 | CNCC | | 35.03 | |  | |  | |  |
|  | -1.00 | OUT | 38 | 25 | 39 | 21 | OCNC | | 9.81 | |  | |  | |  |
| s 104 | 1.00 | TORS | 26 | 22 | 20 | 39 | CCCN | | -51.99 | | f159 17 | | f145 16 | |  |
| s 105 | 1.00 | TORS | 29 | 26 | 22 | 20 | CCCC | | 71.05 | |  | |  | |  |
| s 106 | 1.00 | TORS | 17 | 39 | 20 | 22 | CNCC | | -71.07 | | f1128 11 | |  | |  |
|  | 1.00 | OUT | 38 | 25 | 39 | 21 | OCNC | | 9.81 | |  | |  | |  |
| s 107 | 1.00 | OUT | 36 | 5 | 3 | 4 | OCCC | | 0.34 | | f649 16 | | f382 11 | | f184 10 |
| s 108 | 1.00 | OUT | 13 | 5 | 1 | 6 | CCCC | | 0.65 | | f258 10 | |  | |  |
| s 109 | 1.00 | OUT | 9 | 4 | 2 | 3 | CCCC | | 0.09 | | f382 10 | | f282 14 | | f184 11 |
| s 110 | 1.00 | OUT | 20 | 17 | 21 | 39 | CCCN | | 37.53 | | f339 14 | |  | |  |
| s 111 | -1.00 | OUT | 17 | 2 | 6 | 1 | CCCC | | 2.01 | | f45 58 | |  | |  |
|  | 1.00 | TORS | 6 | 1 | 17 | 39 | CCCN | | 59.95 | |  | |  | |  |

Experimental and calculated wavenumbers of FT-IR spectra of compound 6 by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | IR calculated, scaled ν(cm-1) | IR calculated, unscaled ν(cm-1 | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % |
| 3163 | 3683,74 | 3832,04 | s1 | 100 |  |  |  |  |  |  |
| 3026 | 3024,875 | 3146,65 | s8 | 92 |  |  |  |  |  |  |
| 3003 | 3015,925 | 3137,34 | s7 | 88 |  |  |  |  |  |  |
| - | 3014,839 | 3136,21 | s2 | -89 |  |  |  |  |  |  |
| - | 2989,374 | 3109,72 | s19 | -88 |  |  |  |  |  |  |
| - | 2988,278 | 3108,58 | s4 | 13 | s12 | -81 |  |  |  |  |
| - | 2983,789 | 3103,91 | s4 | 79 | s12 | 12 |  |  |  |  |
| 2976 | 2978,425 | 3098,33 | s16 | 89 |  |  |  |  |  |  |
| - | 2966,351 | 3085,77 | s11 | 94 |  |  |  |  |  |  |
| 2955 | 2955,2 | 3074,17 | s14 | 87 |  |  |  |  |  |  |
| 2945 | 2949,268 | 3068 | s9 | 88 |  |  |  |  |  |  |
| - | 2940,828 | 3059,22 | s5 | 92 |  |  |  |  |  |  |
| - | 2934,243 | 3052,37 | s18 | 80 |  |  |  |  |  |  |
| 2924 | 2927,726 | 3045,59 | s3 | 91 |  |  |  |  |  |  |
| - | 2922,65 | 3040,31 | s17 | 90 |  |  |  |  |  |  |
| - | 2917,18 | 3034,62 | s13 | 96 |  |  |  |  |  |  |
| 2883 | 2907,519 | 3024,57 | s10 | 86 |  |  |  |  |  |  |
| 2874 | 2902,001 | 3018,83 | s6 | 89 |  |  |  |  |  |  |
| 2833 | 2858,608 | 2973,69 | s15 | 97 |  |  |  |  |  |  |
| 1655 | 1675,796 | 1743,26 | s20 | 84 |  |  |  |  |  |  |
| - | 1575,35 | 1638,77 | s24 | 53 |  |  |  |  |  |  |
| 1595 | 1563,324 | 1626,26 | s21 | -55 |  |  |  |  |  |  |
| 1504 | 1476,393 | 1535,83 | s52 | 74 |  |  |  |  |  |  |
| 1496 | 1468,472 | 1527,59 | s45 | 64 |  |  |  |  |  |  |
| 1471 | 1456,85 | 1515,5 | s39 | -14 | s44 | 12 |  |  |  |  |
| 1462 | 1446,17 | 1504,39 | s42 | -69 | s76 | 10 |  |  |  |  |
| - | 1444,882 | 1503,05 | s56 | 85 |  |  |  |  |  |  |
| 1446 | 1439,883 | 1497,85 | s49 | -58 | s74 | 11 |  |  |  |  |
| - | 1436,596 | 1494,43 | s44 | 47 |  |  |  |  |  |  |
| - | 1431,039 | 1488,65 | s50 | 69 | s82 | 11 |  |  |  |  |
| - | 1425,954 | 1483,36 | s46 | -50 | s78 | -10 |  |  |  |  |
| 1423 | 1423,416 | 1480,72 | s40 | -52 |  |  |  |  |  |  |
| 1411 | 1415,985 | 1472,99 | s54 | 85 |  |  |  |  |  |  |
| 1384 | 1390,444 | 1446,42 | s23 | 10 | s26 | -14 | s84 | -12 |  |  |
| 1379 | 1381,109 | 1436,71 | s23 | -22 |  |  |  |  |  |  |
| 1359 | 1367,007 | 1422,04 | s43 | -72 |  |  |  |  |  |  |
| - | 1364,565 | 1419,5 | s48 | 86 |  |  |  |  |  |  |
| 1342 | 1357,038 | 1411,67 | s47 | -76 |  |  |  |  |  |  |
| 1313 | 1336,457 | 1390,26 | s41 | 10 | s87 | -48 |  |  |  |  |
| 1303 | 1294,535 | 1346,65 | s51 | 12 | s55 | 14 | s72 | -47 |  |  |
| 1286 | 1286,421 | 1338,21 | s27 | 38 |  |  |  |  |  |  |
| 1274 | 1274,097 | 1325,39 | s27 | 14 |  |  |  |  |  |  |
| 1251 | 1258,496 | 1309,16 | s23 | 13 | s25 | 16 |  |  |  |  |
| 1249 | 1256,409 | 1306,99 | s55 | -15 | s85 | -51 |  |  |  |  |
| - | 1232,54 | 1282,16 | s38 | -12 | s39 | 10 |  |  |  |  |
| - | 1218,823 | 1267,89 | s39 | 11 | s53 | -13 |  |  |  |  |
| - | 1196,069 | 1244,22 | s28 | -10 | s32 | -19 | s36 | 14 | s39 | 20 |
| 1249 | 1192,646 | 1240,66 | s53 | 42 |  |  |  |  |  |  |
| 1180 | 1175,545 | 1222,87 | s51 | -24 | s85 | 14 | s88 | 12 |  |  |
| - | 1155,771 | 1202,3 | s38 | 22 | s39 | 15 | s41 | -11 |  |  |
| - | 1148,619 | 1194,86 | s38 | 14 | s41 | 12 |  |  |  |  |
| - | 1138,708 | 1184,55 | s51 | 19 | s83 | 13 |  |  |  |  |
| - | 1057,901 | 1100,49 | s78 | -20 |  |  |  |  |  |  |
| 1093 | 1053,335 | 1095,74 | s22 | -16 | s95 | 13 |  |  |  |  |
| - | 1051,701 | 1094,04 | s22 | 22 |  |  |  |  |  |  |
| - | 1027,601 | 1068,97 | s44 | -11 | s77 | 49 |  |  |  |  |
| - | 1025,342 | 1066,62 | s29 | 21 | s80 | -18 |  |  |  |  |
| 1057 | 1011,701 | 1052,43 | s50 | -21 | s82 | -56 |  |  |  |  |
| - | 996,9738 | 1037,11 | s42 | 17 | s76 | -62 |  |  |  |  |
| - | 993,965 | 1033,98 | s80 | -32 |  |  |  |  |  |  |
| - | 985,0826 | 1024,74 | s34 | 51 | s37 | -10 |  |  |  |  |
| 1031 | 974,5948 | 1013,83 | s78 | -22 |  |  |  |  |  |  |
| 1004 | 933,6338 | 971,22 | s73 | -10 |  |  |  |  |  |  |
| 962 | 898,9693 | 935,16 | s35 | 16 | s69 | 36 |  |  |  |  |
| - | 878,5609 | 913,93 | s84 | -13 |  |  |  |  |  |  |
| 931 | 862,536 | 897,26 | s37 | 12 | s73 | 12 |  |  |  |  |
| - | 830,294 | 863,72 | s26 | 20 | s55 | 13 | s69 | 12 |  |  |
| 896 | 814,5479 | 847,34 | s71 | 67 | s97 | 11 |  |  |  |  |
| - | 800,6764 | 832,91 | s22 | -10 | s32 | 17 | s60 | 10 |  |  |
| 852 | 763,3587 | 794,09 | s68 | -13 |  |  |  |  |  |  |
|  | 716,851 | 745,71 | s31 | 12 | s88 | -10 |  |  |  |  |
|  | 690,521 | 718,32 | s28 | 17 |  |  |  |  |  |  |
|  | 646,0417 | 672,05 | s66 | 25 | s97 | -22 |  |  |  |  |
|  | 625,2103 | 650,38 | s37 | 20 | s96 | 23 |  |  |  |  |
|  | 590,0459 | 613,8 | s33 | 10 | s35 | 11 | s66 | -21 | s97 | -12 |
|  | 569,7144 | 592,65 | s62 | -31 | s65 | 10 |  |  |  |  |
|  | 551,8439 | 574,06 | s30 | 41 | s62 | 19 |  |  |  |  |
|  | 542,452 | 564,29 | s86 | 25 | s96 | -30 |  |  |  |  |
|  | 530,1666 | 551,51 | s90 | -59 |  |  |  |  |  |  |
|  | 518,0253 | 538,88 |  |  |  |  |  |  |  |  |
|  | 470,8255 | 489,78 | s57 | 54 |  |  |  |  |  |  |
|  | 441,0829 | 458,84 | s59 | 54 |  |  |  |  |  |  |
|  | 413,2821 | 429,92 | s67 | 56 | s73 | -12 |  |  |  |  |
|  | 360,699 | 375,22 | s91 | 40 |  |  |  |  |  |  |
|  | 332,3214 | 345,7 | s63 | 75 |  |  |  |  |  |  |
|  | 327,3034 | 340,48 | s64 | 54 |  |  |  |  |  |  |
|  | 312,807 | 325,4 | s65 | -20 | s99 | 44 |  |  |  |  |
|  | 305,1647 | 317,45 | s65 | 29 | s99 | 42 |  |  |  |  |
|  | 278,3444 | 289,55 | s70 | -58 |  |  |  |  |  |  |
|  | 228,6164 | 237,82 | s68 | -10 | s101 | -34 |  |  |  |  |
|  | 198,8257 | 206,83 | s98 | 42 | s101 | 11 |  |  |  |  |
|  | 190,9911 | 198,68 | s61 | 43 | s67 | 13 |  |  |  |  |
|  | 165,8339 | 172,51 | s88 | -12 | s95 | 12 | s100 | -11 |  |  |
|  | 144,3104 | 150,12 | s79 | -13 | s86 | 12 | s95 | 15 |  |  |
|  | 135,6298 | 141,09 | s79 | -12 | s100 | -21 |  |  |  |  |
|  | 125,5169 | 130,57 | s81 | 43 | s98 | -13 |  |  |  |  |
|  | 113,6833 | 118,26 | s79 | 30 | s94 | 32 |  |  |  |  |
|  | 100,2732 | 104,31 | s93 | -36 | s100 | -13 |  |  |  |  |
|  | 79,60525 | 82,81 | s81 | -22 | s93 | 15 |  |  |  |  |
|  | 47,72855 | 49,65 | s92 | 62 |  |  |  |  |  |  |
|  | 39,15375 | 40,73 | s68 | -19 | s89 | 54 |  |  |  |  |
|  | 22,1868 | 23,08 | s102 | 65 |  |  |  |  |  |  |

Scaling factor = 0.9613, (-)PED% - asymmetric vibrations

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| s 1 | 1.00 | STRE | 33 | 34 | OH | 0.963501 | | f3832 100 | |  | |  | |
| s 2 | 1.00 | STRE | 5 | 7 | CH | 1.086520 | | f3136 89 | |  | |  | |
|  | -1.00 |  | 11 | 14 | CH | 1.087221 | |  | |  | |  | |
| s 3 | 1.00 | STRE | 8 | 9 | CH | 1.092195 | | f3046 91 | |  | |  | |
| s 4 | 1.00 | STRE | 8 | 10 | CH | 1.089348 | | f3109 13 | | f3104 79 | |  | |
| s 5 | 1.00 | STRE | 11 | 12 | CH | 1.094769 | | f3059 92 | |  | |  | |
|  | -1.00 |  | 11 | 13 | CH | 1.093323 | |  | |  | |  | |
| s 6 | 1.00 | STRE | 11 | 12 | CH | 1.094769 | | f3019 89 | |  | |  | |
|  | 1.00 |  | 11 | 13 | CH | 1.093323 | |  | |  | |  | |
| s 7 | 1.00 | STRE | 5 | 7 | CH | 1.086520 | | f3137 88 | |  | |  | |
|  | 1.00 |  | 11 | 14 | CH | 1.087221 | |  | |  | |  | |
| s 8 | 1.00 | STRE | 15 | 16 | CH | 1.085853 | | f3147 92 | |  | |  | |
| s 9 | 1.00 | STRE | 15 | 17 | CH | 1.094782 | | f3068 88 | |  | |  | |
|  | -1.00 |  | 15 | 18 | CH | 1.092509 | |  | |  | |  | |
| s 10 | 1.00 | STRE | 15 | 17 | CH | 1.094782 | | f3025 86 | |  | |  | |
|  | 1.00 |  | 15 | 18 | CH | 1.092509 | |  | |  | |  | |
| s 11 | 1.00 | STRE | 19 | 20 | CH | 1.093343 | | f3086 94 | |  | |  | |
|  | -1.00 |  | 19 | 22 | CH | 1.090589 | |  | |  | |  | |
| s 12 | -1.00 | STRE | 19 | 21 | CH | 1.090829 | | f3109 81 | | f3104 12 | |  | |
|  | 1.00 |  | 19 | 22 | CH | 1.090589 | |  | |  | |  | |
| s 13 | 1.00 | STRE | 19 | 20 | CH | 1.093343 | | f3035 96 | |  | |  | |
|  | 1.00 |  | 19 | 21 | CH | 1.090829 | |  | |  | |  | |
| s 14 | 1.00 | STRE | 24 | 27 | CH | 1.091046 | | f3074 87 | |  | |  | |
| s 15 | 1.00 | STRE | 24 | 28 | CH | 1.098654 | | f2974 97 | |  | |  | |
| s 16 | 1.00 | STRE | 25 | 29 | CH | 1.089343 | | f3098 89 | |  | |  | |
|  | -1.00 |  | 26 | 31 | CH | 1.091752 | |  | |  | |  | |
|  | 1.00 |  | 26 | 32 | CH | 1.089803 | |  | |  | |  | |
| s 17 | 1.00 | STRE | 25 | 30 | CH | 1.094371 | | f3040 90 | |  | |  | |
| s 18 | 1.00 | STRE | 26 | 31 | CH | 1.091752 | | f3052 80 | |  | |  | |
|  | 1.00 |  | 26 | 32 | CH | 1.089803 | |  | |  | |  | |
| s 19 | 1.00 | STRE | 25 | 29 | CH | 1.089343 | | f3110 88 | |  | |  | |
|  | -1.00 |  | 26 | 32 | CH | 1.089803 | |  | |  | |  | |
| s 20 | 1.00 | STRE | 35 | 23 | OC | 1.218847 | | f1743 84 | |  | |  | |
| s 21 | 1.00 | STRE | 5 | 6 | CC | 1.387968 | | f1626 55 | |  | |  | |
|  | -1.00 |  | 3 | 4 | CC | 1.393325 | |  | |  | |  | |
| s 22 | 1.00 | STRE | 33 | 4 | OC | 1.374656 | | f1096 15 | | f1094 22 | | f833 10 | |
| s 23 | -1.00 | STRE | 1 | 2 | CC | 1.408042 | | f1446 10 | | f1437 22 | | f1309 13 | |
|  | 1.00 |  | 4 | 5 | CC | 1.389858 | |  | |  | |  | |
| s 24 | 1.00 | STRE | 4 | 5 | CC | 1.389858 | | f1639 53 | |  | |  | |
|  | -1.00 |  | 3 | 4 | CC | 1.393325 | |  | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.408042 | |  | |  | |  | |
| s 25 | 1.00 | STRE | 3 | 2 | CC | 1.408615 | | f1309 16 | |  | |  | |
| s 26 | 1.00 | STRE | 36 | 23 | NC | 1.368323 | | f1446 14 | | f864 20 | |  | |
| s 27 | 1.00 | STRE | 5 | 6 | CC | 1.387968 | | f1338 38 | | f1325 14 | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.408042 | |  | |  | |  | |
|  | 1.00 |  | 3 | 4 | CC | 1.393325 | |  | |  | |  | |
| s 28 | 1.00 | STRE | 11 | 3 | CC | 1.508717 | | f1244 10 | | f718 17 | |  | |
| s 29 | 1.00 | STRE | 2 | 15 | CC | 1.513536 | | f1067 21 | |  | |  | |
|  | -1.00 |  | 6 | 19 | CC | 1.509841 | |  | |  | |  | |
| s 30 | 1.00 | STRE | 33 | 4 | OC | 1.374656 | | f574 42 | |  | |  | |
|  | 1.00 |  | 6 | 19 | CC | 1.509841 | |  | |  | |  | |
|  | 1.00 |  | 2 | 15 | CC | 1.513536 | |  | |  | |  | |
|  | 1.00 |  | 1 | 2 | CC | 1.408042 | |  | |  | |  | |
|  | 1.00 |  | 3 | 4 | CC | 1.393325 | |  | |  | |  | |
|  | 1.00 |  | 5 | 6 | CC | 1.387968 | |  | |  | |  | |
| s 31 | 1.00 | STRE | 36 | 24 | NC | 1.458212 | | f746 12 | |  | |  | |
| s 32 | 1.00 | STRE | 8 | 1 | CC | 1.517880 | | f1244 19 | | f833 17 | |  | |
| s 33 | 1.00 | STRE | 36 | 8 | NC | 1.462433 | | f614 10 | |  | |  | |
| s 34 | 1.00 | STRE | 25 | 26 | CC | 1.534017 | | f1025 51 | |  | |  | |
| s 35 | 1.00 | STRE | 23 | 25 | CC | 1.525602 | | f935 16 | | f614 11 | |  | |
|  | 1.00 |  | 25 | 26 | CC | 1.534017 | |  | |  | |  | |
| s 36 | 1.00 | BEND | 1 | 2 | 3 | CCC | 120.93 | | f1244 14 | |  | |  | |  |  |
| s 37 | 1.00 | BEND | 26 | 25 | 23 | CCC | 104.44 | | f1025 10 | | f897 12 | | f650 20 | |  |  |
| s 38 | 1.00 | BEND | 34 | 33 | 4 | HOC | 109.07 | | f1282 12 | | f1202 22 | | f1195 14 | |  |  |
| s 39 | 1.00 | BEND | 7 | 5 | 6 | HCC | 119.49 | | f1516 15 | | f1282 10 | | f1268 11 | | f1244 20 f1202 15 | |
| s 40 | -1.00 | BEND | 20 | 19 | 22 | HCH | 107.63 | | f1481 52 | |  | |  | |  |  |
|  | -1.00 |  | 12 | 11 | 13 | HCH | 106.88 | |  | |  | |  | |  |  |
|  | 1.00 |  | 20 | 19 | 21 | HCH | 106.39 | |  | |  | |  | |  |  |
|  | -1.00 |  | 16 | 15 | 18 | HCH | 107.28 | |  | |  | |  | |  |  |
| s 41 | 1.00 | BEND | 10 | 8 | 1 | HCC | 110.68 | | f1390 10 | | f1202 11 | | f1195 12 | |  |  |
| s 42 | -1.00 | BEND | 13 | 11 | 14 | HCH | 108.04 | | f1504 69 | | f1037 17 | |  | |  |  |
|  | 1.00 |  | 12 | 11 | 14 | HCH | 107.70 | |  | |  | |  | |  |  |
|  | -1.00 |  | 16 | 15 | 17 | HCH | 107.40 | |  | |  | |  | |  |  |
|  | 1.00 |  | 16 | 15 | 18 | HCH | 107.28 | |  | |  | |  | |  |  |
| s 43 | -1.00 | BEND | 12 | 11 | 13 | HCH | 106.88 | | f1422 72 | |  | |  | |  |  |
|  | -1.00 |  | 17 | 15 | 18 | HCH | 106.52 | |  | |  | |  | |  |  |
|  | -1.00 |  | 20 | 19 | 21 | HCH | 106.39 | |  | |  | |  | |  |  |
|  | -1.00 |  | 16 | 15 | 17 | HCH | 107.40 | |  | |  | |  | |  |  |
|  | -1.00 |  | 12 | 11 | 14 | HCH | 107.70 | |  | |  | |  | |  |  |
|  | 1.00 |  | 9 | 8 | 10 | HCH | 106.28 | |  | |  | |  | |  |  |
|  | -1.00 |  | 13 | 11 | 14 | HCH | 108.04 | |  | |  | |  | |  |  |
| s 44 | -1.00 | BEND | 13 | 11 | 14 | HCH | 108.04 | | f1516 12 | | f1494 47 | | f1069 11 | |  |  |
|  | 1.00 |  | 12 | 11 | 13 | HCH | 106.88 | |  | |  | |  | |  |  |
|  | 1.00 |  | 20 | 19 | 22 | HCH | 107.63 | |  | |  | |  | |  |  |
|  | -1.00 |  | 16 | 15 | 18 | HCH | 107.28 | |  | |  | |  | |  |  |
|  | -1.00 |  | 20 | 19 | 21 | HCH | 106.39 | |  | |  | |  | |  |  |
|  | 1.00 |  | 12 | 11 | 14 | HCH | 107.70 | |  | |  | |  | |  |  |
|  | 1.00 |  | 17 | 15 | 18 | HCH | 106.52 | |  | |  | |  | |  |  |
|  | 1.00 |  | 21 | 19 | 22 | HCH | 108.10 | |  | |  | |  | |  |  |
|  | 1.00 |  | 16 | 15 | 17 | HCH | 107.40 | |  | |  | |  | |  |  |
|  | 1.00 |  | 9 | 8 | 10 | HCH | 106.28 | |  | |  | |  | |  |  |
| s 45 | 1.00 | BEND | 9 | 8 | 10 | HCH | 106.28 | | f1528 64 | |  | |  | |  |  |
|  | 1.00 |  | 16 | 15 | 18 | HCH | 107.28 | |  | |  | |  | |  |  |
| s 46 | 1.00 | BEND | 16 | 15 | 17 | HCH | 107.40 | | f1483 50 | |  | |  | |  |  |
|  | -1.00 |  | 17 | 15 | 18 | HCH | 106.52 | |  | |  | |  | |  |  |
|  | -1.00 |  | 13 | 11 | 14 | HCH | 108.04 | |  | |  | |  | |  |  |
| s 47 | -1.00 | BEND | 12 | 11 | 13 | HCH | 106.88 | | f1412 76 | |  | |  | |  |  |
|  | 1.00 |  | 17 | 15 | 18 | HCH | 106.52 | |  | |  | |  | |  |  |
| s 48 | 1.00 | BEND | 20 | 19 | 21 | HCH | 106.39 | | f1420 86 | |  | |  | |  |  |
|  | 1.00 |  | 20 | 19 | 22 | HCH | 107.63 | |  | |  | |  | |  |  |
|  | 1.00 |  | 21 | 19 | 22 | HCH | 108.10 | |  | |  | |  | |  |  |
| s 49 | -1.00 | BEND | 12 | 11 | 14 | HCH | 107.70 | | f1498 58 | |  | |  | |  |  |
|  | 1.00 |  | 20 | 19 | 21 | HCH | 106.39 | |  | |  | |  | |  |  |
|  | 1.00 |  | 12 | 11 | 13 | HCH | 106.88 | |  | |  | |  | |  |  |
|  | -1.00 |  | 21 | 19 | 22 | HCH | 108.10 | |  | |  | |  | |  |  |
|  | -1.00 |  | 20 | 19 | 22 | HCH | 107.63 | |  | |  | |  | |  |  |
| s 50 | 1.00 | BEND | 21 | 19 | 22 | HCH | 108.10 | | f1489 69 | | f1052 21 | |  | |  |  |
|  | -1.00 |  | 20 | 19 | 22 | HCH | 107.63 | |  | |  | |  | |  |  |
| s 51 | 1.00 | BEND | 27 | 24 | 26 | HCC | 112.77 | | f1347 12 | | f1223 25 | | f1185 18 | |  |  |
|  | -1.00 |  | 29 | 25 | 26 | HCC | 114.53 | |  | |  | |  | |  |  |
| s 52 | 1.00 | BEND | 28 | 24 | 27 | HCH | 107.79 | | f1536 74 | |  | |  | |  |  |
| s 53 | 1.00 | BEND | 29 | 25 | 26 | HCC | 114.53 | | f1268 13 | | f1241 42 | |  | |  |  |
|  | 1.00 |  | 27 | 24 | 26 | HCC | 112.77 | |  | |  | |  | |  |  |
| s 54 | 1.00 | BEND | 30 | 25 | 29 | HCH | 107.34 | | f1473 85 | |  | |  | |  |  |
| s 55 | 1.00 | BEND | 31 | 26 | 25 | HCC | 110.15 | | f1347 14 | | f1307 15 | | f864 13 | |  |  |
| s 56 | 1.00 | BEND | 32 | 26 | 31 | HCH | 107.77 | | f1503 85 | |  | |  | |  |  |
| s 57 | 1.00 | BEND | 25 | 23 | 35 | CCO | 126.46 | | f490 54 | |  | |  | |  |  |
|  | 1.00 |  | 1 | 2 | 3 | CCC | 120.93 | |  | |  | |  | |  |  |
| s 58 | 1.00 | BEND | 6 | 5 | 4 | CCC | 121.18 | |  | |  | |  | |  |  |
| s 59 | 1.00 | BEND | 2 | 3 | 4 | CCC | 118.32 | | f459 54 | |  | |  | |  |  |
| s 60 | 1.00 | BEND | 2 | 3 | 4 | CCC | 118.32 | | f833 11 | |  | |  | |  |  |
|  | 1.00 |  | 3 | 4 | 5 | CCC | 120.97 | |  | |  | |  | |  |  |
| s 61 | 1.00 | BEND | 23 | 36 | 8 | CNC | 122.16 | | f199 44 | |  | |  | |  |  |
| s 62 | 1.00 | BEND | 5 | 4 | 33 | CCO | 120.92 | | f593 31 | | f574 19 | |  | |  |  |
|  | -1.00 |  | 1 | 2 | 15 | CCC | 122.31 | |  | |  | |  | |  |  |
|  | 1.00 |  | 2 | 1 | 8 | CCC | 122.14 | |  | |  | |  | |  |  |
|  | -1.00 |  | 2 | 3 | 11 | CCC | 121.66 | |  | |  | |  | |  |  |
| s 63 | 1.00 | BEND | 2 | 3 | 11 | CCC | 121.66 | | f346 75 | |  | |  | |  |  |
|  | 1.00 |  | 5 | 4 | 33 | CCO | 120.92 | |  | |  | |  | |  |  |
| s 64 | 1.00 | BEND | 1 | 2 | 15 | CCC | 122.31 | | f341 54 | |  | |  | |  |  |
|  | 1.00 |  | 5 | 4 | 33 | CCO | 120.92 | |  | |  | |  | |  |  |
|  | -1.00 |  | 2 | 1 | 8 | CCC | 122.14 | |  | |  | |  | |  |  |
| s 65 | 1.00 | BEND | 19 | 6 | 5 | CCC | 118.80 | | f593 10 | | f325 21 f | | 317 29 | |  |  |
| s 66 | 1.00 | BEND | 23 | 36 | 24 | CNC | 113.33 | | f672 25 | | f614 21 | |  | |  |  |
|  | -1.00 |  | 25 | 23 | 36 | CCN | 107.81 | |  | |  | |  | |  |  |
| s 67 | 1.00 | BEND | 2 | 1 | 8 | CCC | 122.14 | | f430 56 | | f199 13 | |  | |  |  |
|  | 1.00 |  | 1 | 2 | 15 | CCC | 122.31 | |  | |  | |  | |  |  |
| s 68 | 1.00 | BEND | 36 | 8 | 1 | NCC | 113.95 | | f794 14 | | f238 10 f | | 173 10 f | | 41 15 |  |
| s 69 | 1.00 | BEND | 23 | 36 | 24 | CNC | 113.33 | | f935 36 | | f864 12 | |  | |  |  |
|  | 1.00 |  | 25 | 23 | 36 | CCN | 107.81 | |  | |  | |  | |  |  |
| s 70 | 1.00 | OUT | 11 | 2 | 4 | 3 | CCCC | | | 0.04 | f290 62 | |  | |  | |
|  | 1.00 |  | 15 | 1 | 3 | 2 | CCCC | | | 0.33 |  | |  | |  | |
|  | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | | 0.15 |  | |  | |  | |
|  | 1.00 | OUT | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
| s 71 | 1.00 | TORS | 7 | 5 | 6 | 19 | HCCC | | | -0.77 | f847 67 | |  | |  | |
| s 72 | 1.00 | TORS | 31 | 26 | 25 | 23 | HCCC | | | -93.41 | f1347 47 | |  | |  | |
|  | -1.00 |  | 32 | 26 | 25 | 23 | HCCC | | | -214.42 |  | |  | |  | |
| s 73 | 1.00 | TORS | 9 | 8 | 1 | 6 | HCCC | | | -155.46 | f971 10 | | f897 12 | | f430 12 | |
| s 74 | 1.00 | TORS | 12 | 11 | 3 | 4 | HCCC | | | -114.69 | f1498 11 | |  | |  | |
| s 75 | 1.00 | TORS | 13 | 11 | 3 | 4 | HCCC | | | -234.11 |  | |  | |  | |
| s 76 | -1.00 | TORS | 16 | 15 | 2 | 3 | HCCC | | | -170.39 | f1504 10 | | f1037 62 | |  | |
|  | 1.00 |  | 18 | 15 | 2 | 3 | HCCC | | | -49.66 |  | |  | |  | |
| s 77 | 1.00 | TORS | 14 | 11 | 3 | 4 | HCCC | | | 5.43 | f1069 49 | |  | |  | |
|  | -1.00 |  | 18 | 15 | 2 | 3 | HCCC | | | -49.66 |  | |  | |  | |
|  | 1.00 |  | 16 | 15 | 2 | 3 | HCCC | | | -170.39 |  | |  | |  | |
| s 78 | 1.00 | TORS | 17 | 15 | 2 | 3 | HCCC | | | 68.58 | f1483 10 | | f1101 19 | | f1014 23 | |
|  | -1.00 |  | 18 | 15 | 2 | 3 | HCCC | | | -49.66 |  | |  | |  | |
| s 79 | -1.00 | TORS | 21 | 19 | 6 | 5 | HCCC | | | -235.62 | f150 13 | | f141 12 | | f118 28 | |
|  | -1.00 |  | 20 | 19 | 6 | 5 | HCCC | | | -116.23 |  | |  | |  | |
|  | 1.00 |  | 17 | 15 | 2 | 3 | HCCC | | | 68.58 |  | |  | |  | |
| s 80 | -1.00 | TORS | 21 | 19 | 6 | 5 | HCCC | | | -235.62 | f1067 18 | | f1034 32 | |  | |
|  | 1.00 |  | 20 | 19 | 6 | 5 | HCCC | | | -116.23 |  | |  | |  | |
| s 81 | 1.00 | TORS | 17 | 15 | 2 | 3 | HCCC | | | 68.58 | f131 44 | | f83 22 | |  | |
|  | 1.00 |  | 20 | 19 | 6 | 5 | HCCC | | | -116.23 |  | |  | |  | |
|  | 1.00 |  | 21 | 19 | 6 | 5 | HCCC | | | -235.62 |  | |  | |  | |
| s 82 | 1.00 | TORS | 22 | 19 | 6 | 5 | HCCC | | | 3.57 | f1489 11 | | f1052 56 | |  | |
| s 83 | 1.00 | TORS | 27 | 24 | 36 | 8 | HCNC | | | -52.30 | f1185 13 | |  | |  | |
| s 84 | 1.00 | TORS | 28 | 24 | 36 | 8 | HCNC | | | 67.18 | f1446 12 | | f914 13 | |  | |
| s 85 | -1.00 | TORS | 30 | 25 | 23 | 36 | HCCN | | | -252.63 | f1307 51 | | f1223 14 | |  | |
|  | 1.00 |  | 29 | 25 | 23 | 36 | HCCN | | | -135.78 |  | |  | |  | |
| s 86 | 1.00 | TORS | 29 | 25 | 23 | 36 | HCCN | | | -135.78 | f564 25 | | f150 12 | |  | |
| s 87 | 1.00 | TORS | 10 | 8 | 1 | 6 | HCCC | | | -37.64 | f1390 48 | |  | |  | |
|  | -1.00 |  | 9 | 8 | 1 | 6 | HCCC | | | -155.46 |  | |  | |  | |
| s 88 | 1.00 | TORS | 32 | 26 | 25 | 23 | HCCC | | | -214.42 | f1223 12 | | f746 10 | | f173 11 | |
| s 89 | 1.00 | OUT | 8 | 2 | 6 | 1 | CCCC | | | 0.66 | f41 56 | |  | |  | |
|  | -1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | | -0.85 |  | |  | |  | |
|  | 1.00 |  | 1 | 8 | 36 | 23 | CCNC | | | -133.46 |  | |  | |  | |
|  | -1.00 |  | 2 | 3 | 4 | 5 | CCCC | | | 0.55 |  | |  | |  | |
|  | 1.00 |  | 8 | 36 | 23 | 25 | CNCC | | | -171.65 |  | |  | |  | |
| s 90 | -1.00 | OUT | 15 | 1 | 3 | 2 | CCCC | | | 0.33 | f551 51 | |  | |  | |
|  | -1.00 |  | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
|  | 1.00 | TORS | 2 | 3 | 4 | 5 | CCCC | | | 0.55 |  | |  | |  | |
|  | 1.00 |  | 3 | 4 | 5 | 6 | CCCC | | | 0.15 |  | |  | |  | |
| s 91 | -1.00 | OUT | 8 | 2 | 6 | 1 | CCCC | | | 0.66 | f375 46 | |  | |  | |
|  | -1.00 |  | 11 | 2 | 4 | 3 | CCCC | | | 0.04 |  | |  | |  | |
|  | -1.00 |  | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
|  | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | | 0.15 |  | |  | |  | |
|  | -1.00 | OUT | 33 | 3 | 5 | 4 | OCCC | | | 0.01 |  | |  | |  | |
| s 92 | 1.00 | TORS | 1 | 8 | 36 | 23 | CCNC | | | -133.46 | f50 59 | |  | |  | |
|  | -1.00 |  | 6 | 1 | 8 | 36 | CCCN | | | 80.70 |  | |  | |  | |
| s 93 | 1.00 | OUT | 11 | 2 | 4 | 3 | CCCC | | | 0.04 | f104 37 | | f83 13 | |  | |
|  | -1.00 |  | 15 | 1 | 3 | 2 | CCCC | | | 0.33 |  | |  | |  | |
|  | -1.00 |  | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
|  | 1.00 | TORS | 1 | 8 | 36 | 23 | CCNC | | | -133.46 |  | |  | |  | |
|  | -1.00 |  | 2 | 3 | 4 | 5 | CCCC | | | 0.55 |  | |  | |  | |
|  | -1.00 |  | 8 | 36 | 23 | 25 | CNCC | | | -171.65 |  | |  | |  | |
| s 94 | 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | | -0.85 | f118 29 | |  | |  | |
| s 95 | 1.00 | TORS | 26 | 25 | 23 | 36 | CCCN | | | -12.19 | f1096 13 | | f173 12 | | f150 15 | |
| s 96 | 1.00 | OUT | 35 | 25 | 36 | 23 | OCNC | | | 0.59 | f650 23 | | f564 29 | |  | |
| s 97 | -1.00 | OUT | 8 | 2 | 6 | 1 | CCCC | | | 0.66 | f847 10 | | f672 23 | | f614 13 | |
|  | -1.00 |  | 11 | 2 | 4 | 3 | CCCC | | | 0.04 |  | |  | |  | |
|  | 1.00 |  | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
|  | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | | 0.15 |  | |  | |  | |
|  | 1.00 | OUT | 33 | 3 | 5 | 4 | OCCC | | | 0.01 |  | |  | |  | |
| s 98 | 1.00 | OUT | 15 | 1 | 3 | 2 | CCCC | | | 0.33 | f207 42 | | f131 13 | |  | |
|  | -1.00 |  | 19 | 1 | 5 | 6 | CCCC | | | 0.65 |  | |  | |  | |
|  | 1.00 |  | 33 | 3 | 5 | 4 | OCCC | | | 0.01 |  | |  | |  | |
| s 99 | 1.00 | TORS | 34 | 33 | 4 | 3 | HOCC | | | -178.72 | f325 44 | | f317 42 | |  | |
|  | 1.00 | OUT | 11 | 2 | 4 | 3 | CCCC | | | 0.04 |  | |  | |  | |
|  | 1.00 |  | 15 | 1 | 3 | 2 | CCCC | | | 0.33 |  | |  | |  | |
|  | 1.00 | TORS | 3 | 4 | 5 | 6 | CCCC | | | 0.15 |  | |  | |  | |
| s 10 | 0 1.00 | TORS | 1 | 2 | 3 | 4 | CCCC | | | -0.85 | f173 11 | | f141 22 | | f118 11 | |
|  | 1.00 |  | 2 | 3 | 4 | 5 | CCCC | | | 0.55 |  | |  | |  | |
|  | 1.00 |  | 6 | 1 | 8 | 36 | CCCN | | | 80.70 |  | |  | |  | |
|  | -1.00 |  | 8 | 36 | 23 | 25 | CNCC | | | -171.65 |  | |  | |  | |
| s 101 | 1.00 | OUT | 24 | 8 | 23 | 36 | CCCN | | | 12.66 | f238 35 | | f207 11 | |  | |
| s 102 | 01.01.1900 | OUT | 8 | 2 | 6 | 1 | CCCC | | | 0.66 | f23 62 | |  | |  | |
|  | 1.00 | TORS | 1 | 8 | 36 | 23 | CCNC | | | -133.46 |  | |  | |  | |
|  | 1.00 |  | 6 | 1 | 8 | 36 | CCCN | | | 80.70 |  | |  | |  | |

Experimental and calculated wavenumbers of FT-IR spectra of compound 7 by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | | IR calculated, scaled ν(cm-1) | | IR calculated, unscaled ν(cm-1 | | Vibration | | PED, % | | Vibration | | PED, % | | | Vibration | | | PED, % | | | Vibration | | | |
| 3441 | | 3684,23 | | 3832,55 | | s1 | | 100 | |  | |  | | |  | | |  | | |  | | | |
|  | | 3026,893 | | 3148,75 | | s8 | | 90 | |  | |  | | |  | | |  | | |  | | | |
| 3024 | | 3016,194 | | 3137,62 | | s2 | | 93 | |  | |  | | |  | | |  | | |  | | | |
|  | | 3014,204 | | 3135,55 | | s4 | | 86 | |  | |  | | |  | | |  | | |  | | | |
| 3005 | | 3003,793 | | 3124,72 | | s12 | | 91 | |  | |  | | |  | | |  | | |  | | | |
| 2982 | | 2978,377 | | 3098,28 | | s10 | | -18 | | s11 | | 80 | | |  | | |  | | |  | | | |
| 2980 | | 2973,907 | | 3093,63 | | s18 | | 92 | |  | |  | | |  | | |  | | |  | | | |
| 2957 | | 2953,354 | | 3072,25 | | s9 | | 98 | |  | |  | | |  | | |  | | |  | | | |
| 2947 | | 2949,461 | | 3068,2 | | s3 | | -14 | | s6 | | 58 | | | s7 | | | -15 | | |  | | | |
| - | | 2948,903 | | 3067,62 | | s16 | | 65 | |  | |  | | |  | | |  | | |  | | | |
| - | | 2945,692 | | 3064,28 | | s17 | | -79 | |  | |  | | |  | | |  | | |  | | | |
| - | | 2944,654 | | 3063,2 | | s3 | | 78 | | s6 | | 14 | | |  | | |  | | |  | | | |
| 2936 | | 2941,857 | | 3060,29 | | s16 | | -13 | | s20 | | -10 | | | s21 | | | 71 | | |  | | | |
| - | | 2937,483 | | 3055,74 | | s13 | | 89 | |  | |  | | |  | | |  | | |  | | | |
| - | | 2908,817 | | 3025,92 | | s10 | | 81 | | s11 | | 17 | | |  | | |  | | |  | | | |
| - | | 2908,634 | | 3025,73 | | s19 | | 65 | | s21 | | -14 | | |  | | |  | | |  | | | |
| 2924 | | 2905,731 | | 3022,71 | | s15 | | 77 | |  | |  | | |  | | |  | | |  | | | |
| 2924 | | 2905,385 | | 3022,35 | | s5 | | 87 | |  | |  | | |  | | |  | | |  | | | |
| 2920 | | 2903,578 | | 3020,47 | | s6 | | 17 | | s7 | | 77 | | |  | | |  | | |  | | | |
| 2901 | | 2894,945 | | 3011,49 | | s19 | | 14 | | s20 | | 76 | | |  | | |  | | |  | | | |
| 2872 | | 2846,486 | | 2961,08 | | s14 | | 97 | |  | |  | | |  | | |  | | |  | | | |
| 1608 | | 1625,856 | | 1691,31 | | s22 | | 83 | |  | |  | | |  | | |  | | |  | | | |
| 1591 | | 1574,225 | | 1637,6 | | s27 | | -44 | |  | |  | | |  | | |  | | |  | | | |
| 1560 | | 1561,478 | | 1624,34 | | s26 | | 58 | |  | |  | | |  | | |  | | |  | | | |
| 1496 | | 1470,078 | | 1529,26 | | s48 | | 14 | | s53 | | 23 | | | s55 | | | -19 | | |  | | | |
| 491 | | 1468,54 | | 1527,66 | | s53 | | 13 | | s55 | | 47 | | |  | | |  | | |  | | | |
| 1475 | | 1460,984 | | 1519,8 | | s42 | | -11 | | s44 | | 18 | | | s53 | | | 17 | | |  | | | |
| 1462 | | 1454,187 | | 1512,73 | | s47 | | -67 | |  | |  | | |  | | |  | | |  | | | |
| 1458 | | 1444,776 | | 1502,94 | | s57 | | 51 | |  | |  | | |  | | |  | | |  | | | |
| 1450 | | 1443,421 | | 1501,53 | | s45 | | 59 | |  | |  | | |  | | |  | | |  | | | |
| 1446 | | 1440,845 | | 1498,85 | | s44 | | 40 | |  | |  | | |  | | |  | | |  | | | |
| 1442 | | 1435,644 | | 1493,44 | | s61 | | 80 | |  | |  | | |  | | |  | | |  | | | |
| 1438 | | 1433,106 | | 1490,8 | | s51 | | 56 | |  | |  | | |  | | |  | | |  | | | |
| - | | 1430,549 | | 1488,14 | | s50 | | 57 | |  | |  | | |  | | |  | | |  | | | |
| - | | 1427,396 | | 1484,86 | | s48 | | 36 | | s51 | | 10 | | | s53 | | | -15 | | |  | | | |
| 1417 | | 1417,773 | | 1474,85 | | s28 | | 10 | | s59 | | 42 | | | s90 | | | 11 | | |  | | | |
| 1411 | | 1401,374 | | 1457,79 | | s59 | | 34 | | s90 | | -14 | | |  | | |  | | |  | | | |
| 1384 | | 1381,167 | | 1436,77 | | s65 | | 14 | | s68 | | 13 | | |  | | |  | | |  | | | |
| 1377 | | 1372,765 | | 1428,03 | | s43 | | 81 | |  | |  | | |  | | |  | | |  | | | |
| 1369 | | 1364,354 | | 1419,28 | | s49 | | 92 | |  | |  | | |  | | |  | | |  | | | |
| - | | 1361,355 | | 1416,16 | | s46 | | 67 | |  | |  | | |  | | |  | | |  | | | |
| 1363 | | 1335,082 | | 1388,83 | | s91 | | -56 | |  | |  | | |  | | |  | | |  | | | |
| 1357 | | 1332,516 | | 1386,16 | | s87 | | -50 | |  | |  | | |  | | |  | | |  | | | |
| 1350 | | 1326,286 | | 1379,68 | | s95 | | 37 | |  | |  | | |  | | |  | | |  | | | |
| 1330 | | 1310,31 | | 1363,06 | | s56 | | 20 | |  | |  | | |  | | |  | | |  | | | |
| 1327 | | 1302,062 | | 1354,48 | | s60 | | 15 | | s94 | | 20 | | |  | | |  | | |  | | | |
| 1321 | | 1276,203 | | 1327,58 | | s31 | | -51 | |  | |  | | |  | | |  | | |  | | | |
| 1315 | | 1268,253 | | 1319,31 | | s29 | | -53 | |  | |  | | |  | | |  | | |  | | | |
| 1305 | | 1257,179 | | 1307,79 | | s54 | | 36 | |  | |  | | |  | | |  | | |  | | | |
| 1278 | | 1240,279 | | 1290,21 | | s58 | | 29 | | s93 | | 10 | | |  | | |  | | |  | | | |
| 1259 | | 1232,444 | | 1282,06 | | s54 | | -11 | | s58 | | 10 | | | s94 | | | 11 | | |  | | | |
| 1242 | | 1212,392 | | 1261,2 | |  | |  | |  | |  | | |  | | |  | | |  | | | |
| 1215 | | 1193,925 | | 1241,99 | | s25 | | 32 | | s42 | | 23 | | |  | | |  | | |  | | | |
| 1184 | | 1155,108 | | 1201,61 | | s27 | | -11 | | s41 | | 35 | | | s42 | | | 13 | | |  | | | |
| 1182 | | 1152,503 | | 1198,9 | | s89 | | 10 | |  | |  | | |  | | |  | | |  | | | |
| 1174 | | 1143,063 | | 1189,08 | | s60 | | -10 | |  | |  | | |  | | |  | | |  | | | |
| 1163 | | 1131,181 | | 1176,72 | | s34 | | 10 | | s37 | | -14 | | | s52 | | | 12 | | |  | | | |
| 1107 | | 1073,513 | | 1116,73 | | s60 | | -13 | | s103 | | -19 | | |  | | |  | | |  | | | |
| 1095 | | 1062,794 | | 1105,58 | | s35 | | -13 | | s38 | | 13 | | |  | | |  | | |  | | | |
| 1089 | | 1059,843 | | 1102,51 | | s23 | | 21 | | s48 | | -10 | | | s81 | | | -12 | | | s82 | | | |
| 1085 | | 1048,009 | | 1090,2 | | s24 | | 48 | |  | |  | | |  | | |  | | |  | | | |
| 1066 | | 1031,571 | | 1073,1 | | s34 | | -27 | | s79 | | 24 | | |  | | |  | | |  | | | |
| 1062 | | 1028,764 | | 1070,18 | | s34 | | 21 | | s79 | | 20 | | |  | | |  | | |  | | | |
| 1041 | | 1015,892 | | 1056,79 | | s51 | | -19 | | s86 | | -53 | | |  | | |  | | |  | | | |
| 1030 | | 1011,864 | | 1052,6 | | s30 | | 13 | | s85 | | 29 | | |  | | |  | | |  | | | |
| 1018 | | 999,3194 | | 1039,55 | | s47 | | 14 | | s83 | | 60 | | |  | | |  | | |  | | | |
| 1004 | | 985,3325 | | 1025 | | s85 | | -21 | |  | |  | | |  | | |  | | |  | | | |
| 983 | | 957,003 | | 995,53 | | s36 | | 10 | | s72 | | -11 | | |  | | |  | | |  | | | |
| 962 | | 938,2288 | | 976 | | s72 | | -10 | |  | |  | | |  | | |  | | |  | | | |
| 925 | | 905,8426 | | 942,31 | | s96 | | 10 | | s102 | | -16 | | |  | | |  | | |  | | | |
| 920 | | 895,7778 | | 931,84 | | s30 | | 13 | | s96 | | 12 | | |  | | |  | | |  | | | |
| 889 | | 862,2861 | | 897 | | s38 | | -10 | | s88 | | 16 | | |  | | |  | | |  | | | |
| 885 | | 851,5292 | | 885,81 | | s36 | | 45 | |  | |  | | |  | | |  | | |  | | | |
| 860 | | 814,9613 | | 847,77 | | s23 | | 19 | |  | |  | | |  | | |  | | |  | | | |
| 854 | | 808,511 | | 841,06 | | s77 | | 61 | |  | |  | | |  | | |  | | |  | | | |
| 846 | | 805,1272 | | 837,54 | | s92 | | 10 | |  | |  | | |  | | |  | | |  | | | |
| 775 | | 741,7968 | | 771,66 | | s98 | | -18 | |  | |  | | |  | | |  | | |  | | | |
| 717 | | 693,328 | | 721,24 | | s28 | | 13 | | s37 | | 17 | | | s98 | | | -15 | | |  | | | |
| 704 | | 682,5518 | | 710,03 | | s33 | | 14 | | s65 | | 16 | | |  | | |  | | |  | | | |
| 661 | | 642,5618 | | 668,43 | | s37 | | -10 | | s73 | | 10 | | | s96 | | | -11 | | | s105 | | | |
|  | | 617,9813 | | 642,86 | | s105 | | 12 | | s107 | | 14 | | |  | | |  | | |  | | | |
|  | | 570,5508 | | 593,52 | | s69 | | -40 | |  | |  | | |  | | |  | | |  | | | |
|  | | 556,3139 | | 578,71 | | s32 | | 53 | | s69 | | 10 | | |  | | |  | | |  | | | |
|  | | 545,6243 | | 567,59 | | s93 | | 14 | | s105 | | -16 | | |  | | |  | | |  | | | |
|  | | 531,2913 | | 552,68 | | s108 | | -64 | |  | |  | | |  | | |  | | |  | | | |
|  | | 527,1673 | | 548,39 | | s75 | | -12 | | s107 | | -15 | | |  | | |  | | |  | | | |
|  | | 491,032 | | 510,8 | | s62 | | 44 | |  | |  | | |  | | |  | | |  | | | |
|  | | 453,3779 | | 471,63 | | s63 | | -23 | |  | |  | | |  | | |  | | |  | | | |
|  | | 446,5046 | | 464,48 | | s40 | | 29 | | s72 | | 12 | | |  | | |  | | |  | | | |
|  | | 435,9688 | | 453,52 | | s63 | | -10 | |  | |  | | |  | | |  | | |  | | | |
|  | | 380,4633 | | 395,78 | | s71 | | 34 | |  | |  | | |  | | |  | | |  | | | |
|  | | 356,2482 | | 370,59 | | s70 | | -22 | | s107 | | -11 | | |  | | |  | | |  | | | |
|  | | 342,3382 | | 356,12 | | s70 | | 48 | |  | |  | | |  | | |  | | |  | | | |
|  | | 330,0912 | | 343,38 | | s39 | | 71 | |  | |  | | |  | | |  | | |  | | | |
|  | | 311,8649 | | 324,42 | | s67 | | 52 | |  | |  | | |  | | |  | | |  | | | |
|  | | 309,5482 | | 322,01 | | s76 | | -15 | | s92 | | 20 | | | s103 | | | -14 | | |  | | | |
|  | | 300,8196 | | 312,93 | | s76 | | 61 | |  | |  | | |  | | |  | | |  | | | |
|  | | 277,6715 | | 288,85 | | s76 | | -11 | | s109 | | -52 | | |  | | |  | | |  | | | |
|  | | 244,7662 | | 254,62 | | s104 | | 32 | |  | |  | | |  | | |  | | |  | | | |
|  | | 210,0633 | | 218,52 | | s33 | | 10 | | s66 | | 28 | | | s71 | | | -19 | | |  | | | |
|  | | 202,767 | | 210,93 | | s98 | | 10 | | s106 | | 49 | | |  | | |  | | |  | | | |
|  | | 171,3229 | | 178,22 | | s81 | | -10 | | s82 | | -15 | | | s110 | | | -10 | | |  | | | |
|  | | 163,6421 | | 170,23 | | s84 | | 61 | | s106 | | -10 | | |  | | |  | | |  | | | |
|  | | 135,3799 | | 140,83 | | s110 | | 29 | |  | |  | | |  | | |  | | |  | | | |
|  | | 120,3163 | | 125,16 | | s111 | | 36 | |  | |  | | |  | | |  | | |  | | | |
|  | | 108,7519 | | 113,13 | | \* | | 113.68 | | s78 | | -12 | | | s102 | | | 34 | | |  | | | |
|  | | 105,6661 | | 109,92 | | s79 | | -13 | | s102 | | -10 | | | s111 | | | 19 | | |  | | | |
|  | | 93,21726 | | 96,97 | | s97 | | -45 | |  | |  | | |  | | |  | | |  | | | |
|  | | 55,21707 | | 57,44 | | s100 | | -68 | |  | |  | | |  | | |  | | |  | | | |
|  | | 43,53728 | | 45,29 | | s75 | | -18 | | s99 | | 52 | | |  | | |  | | |  | | | |
|  | | 35,52965 | | 36,96 | | s101 | | -66 | |  | |  | | |  | | |  | | |  | | | |
| Scaling factor = 0.9613, (-)PED% - asymmetric vibrations | | | | | | | | | | | | | | | | | | | | | | | | |
| s 1 | 1.00 | | STRE | | 37 | | 38 | | OH | | 0.963444 | | | f3833 100 | | |  | | |  | | |
| s 2 | 1.00 | | STRE | | 5 | | 7 | | CH | | 1.086451 | | | f3138 93 | | |  | | |  | | |
| s 3 | 1.00 | | STRE | | 8 | | 9 | | CH | | 1.094626 | | | f3068 14 | | | f3063 78 | | |  | | |
|  | -1.00 | |  | | 8 | | 11 | | CH | | 1.092959 | | |  | | |  | | |  | | |
| s 4 | 1.00 | | STRE | | 8 | | 10 | | CH | | 1.087354 | | | f3136 86 | | |  | | |  | | |
| s 5 | 1.00 | | STRE | | 8 | | 9 | | CH | | 1.094626 | | | f3022 87 | | |  | | |  | | |
|  | 1.00 | |  | | 8 | | 11 | | CH | | 1.092959 | | |  | | |  | | |  | | |
| s 6 | 1.00 | | STRE | | 12 | | 13 | | CH | | 1.092505 | | | f3068 58 | | | f3063 14 | | | f3020 17 | | |
| s 7 | 1.00 | | STRE | | 12 | | 14 | | CH | | 1.095291 | | | f3068 15 | | | f3020 77 | | |  | | |
| s 8 | 1.00 | | STRE | | 12 | | 15 | | CH | | 1.086189 | | | f3149 90 | | |  | | |  | | |
| s 9 | 1.00 | | STRE | | 16 | | 17 | | CH | | 1.093339 | | | f3072 98 | | |  | | |  | | |
|  | -1.00 | |  | | 16 | | 18 | | CH | | 1.092724 | | |  | | |  | | |  | | |
| s 10 | 1.00 | | STRE | | 16 | | 17 | | CH | | 1.093339 | | | f3098 18 | | | f3026 81 | | |  | | |
|  | 1.00 | |  | | 16 | | 18 | | CH | | 1.092724 | | |  | | |  | | |  | | |
| s 11 | 1.00 | | STRE | | 16 | | 19 | | CH | | 1.090641 | | | f3098 80 | | | f3026 17 | | |  | | |
| s 12 | 1.00 | | STRE | | 20 | | 21 | | CH | | 1.087136 | | | f3125 91 | | |  | | |  | | |
| s 13 | 1.00 | | STRE | | 20 | | 22 | | CH | | 1.091907 | | | f3056 89 | | |  | | |  | | |
| s 14 | 1.00 | | STRE | | 23 | | 26 | | CH | | 1.099905 | | | f2961 97 | | |  | | |  | | |
| s 15 | 1.00 | | STRE | | 25 | | 30 | | CH | | 1.093036 | | | f3023 77 | | |  | | |  | | |
|  | 1.00 | |  | | 25 | | 31 | | CH | | 1.095074 | | |  | | |  | | |  | | |
| s 16 | -1.00 | | STRE | | 25 | | 30 | | CH | | 1.093036 | | | f3068 65 | | | f3060 13 | | |  | | |
|  | 1.00 | |  | | 25 | | 31 | | CH | | 1.095074 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 23 | | 27 | | CH | | 1.091886 | | |  | | |  | | |  | | |
| s 17 | -1.00 | | STRE | | 23 | | 27 | | CH | | 1.091886 | | | f3064 79 | | |  | | |  | | |
|  | -1.00 | |  | | 25 | | 30 | | CH | | 1.093036 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 25 | | 31 | | CH | | 1.095074 | | |  | | |  | | |  | | |
| s 18 | 1.00 | | STRE | | 28 | | 32 | | CH | | 1.090475 | | | f3094 92 | | |  | | |  | | |
| s 19 | 1.00 | | STRE | | 28 | | 33 | | CH | | 1.095832 | | | f3026 65 | | | f3012 14 | | |  | | |
|  | 1.00 | |  | | 25 | | 31 | | CH | | 1.095074 | | |  | | |  | | |  | | |
| s 20 | 1.00 | | STRE | | 29 | | 35 | | CH | | 1.095713 | | | f3060 10 | | | f3012 76 | | |  | | |
| s 21 | 1.00 | | STRE | | 29 | | 34 | | CH | | 1.092935 | | | f3060 71 | | | f3026 14 | | |  | | |
| s 22 | 1.00 | | STRE | | 39 | | 24 | | OC | | 1.226336 | | | f1691 83 | | |  | | |  | | |
| s 23 | -1.00 | | STRE | | 1 | | 20 | | CC | | 1.518220 | | | f1102 21 | | | f848 18 | | |  | | |
|  | 1.00 | |  | | 37 | | 4 | | OC | | 1.374945 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 2 | | 12 | | CC | | 1.511334 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 8 | | CC | | 1.508435 | | |  | | |  | | |  | | |
| s 24 | 1.00 | | STRE | | 4 | | 5 | | CC | | 1.388347 | | | f1090 48 | | |  | | |  | | |
|  | 1.00 | |  | | 37 | | 4 | | OC | | 1.374945 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 6 | | 16 | | CC | | 1.513431 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 1 | | 20 | | CC | | 1.518220 | | |  | | |  | | |  | | |
| s 25 | -1.00 | | STRE | | 1 | | 20 | | CC | | 1.518220 | | | f1242 32 | | |  | | |  | | |
|  | -1.00 | |  | | 3 | | 8 | | CC | | 1.508435 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 5 | | 6 | | CC | | 1.390966 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 1 | | 6 | | CC | | 1.406661 | | |  | | |  | | |  | | |
| s 26 | -1.00 | | STRE | | 5 | | 6 | | CC | | 1.390966 | | | f1624 58 | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 4 | | CC | | 1.395074 | | |  | | |  | | |  | | |
| s 27 | 1.00 | | STRE | | 4 | | 5 | | CC | | 1.388347 | | | f1638 44 | | | f1202 11 | | |  | | |
|  | -1.00 | |  | | 3 | | 4 | | CC | | 1.395074 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 1 | | 6 | | CC | | 1.406661 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 2 | | 3 | | CC | | 1.405716 | | |  | | |  | | |  | | |
| s 28 | 1.00 | | STRE | | 36 | | 24 | | NC | | 1.368731 | | | f1475 10 | | | f721 13 | | |  | | |
| s 29 | -1.00 | | STRE | | 2 | | 3 | | CC | | 1.405716 | | | f1319 53 | | |  | | |  | | |
|  | -1.00 | |  | | 1 | | 6 | | CC | | 1.406661 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 37 | | 4 | | OC | | 1.374945 | | |  | | |  | | |  | | |
| s 30 | 1.00 | | STRE | | 2 | | 12 | | CC | | 1.511334 | | | f1053 12 | | | f932 13 | | |  | | |
|  | -1.00 | |  | | 6 | | 16 | | CC | | 1.513431 | | |  | | |  | | |  | | |
| s 31 | -1.00 | | STRE | | 5 | | 6 | | CC | | 1.390966 | | | f1328 51 | | |  | | |  | | |
|  | 1.00 | |  | | 37 | | 4 | | OC | | 1.374945 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 3 | | 4 | | CC | | 1.395074 | | |  | | |  | | |  | | |
| s 32 | 1.00 | | STRE | | 2 | | 12 | | CC | | 1.511334 | | | f579 53 | | |  | | |  | | |
|  | 1.00 | |  | | 37 | | 4 | | OC | | 1.374945 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 5 | | 6 | | CC | | 1.390966 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 4 | | 5 | | CC | | 1.388347 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 4 | | CC | | 1.395074 | | |  | | |  | | |  | | |
| s 33 | 1.00 | | STRE | | 1 | | 6 | | CC | | 1.406661 | | | f710 14 | | | f219 10 | | |  | | |
|  | 1.00 | |  | | 1 | | 20 | | CC | | 1.518220 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 8 | | CC | | 1.508435 | | |  | | |  | | |  | | |
| s 34 | -1.00 | | STRE | | 25 | | 29 | | CC | | 1.524461 | | | f1177 10 | | | f1073 26 | | | f1070 21 | | |
|  | 1.00 | |  | | 23 | | 25 | | CC | | 1.521588 | | |  | | |  | | |  | | |
| s 35 | 1.00 | | STRE | | 28 | | 24 | | CC | | 1.524778 | | | f1106 13 | | |  | | |  | | |
| s 36 | 1.00 | | STRE | | 25 | | 29 | | CC | | 1.524461 | | | f996 10 | | | f886 45 | | |  | | |
|  | 1.00 | |  | | 23 | | 25 | | CC | | 1.521588 | | |  | | |  | | |  | | |
| s 37 | 1.00 | | STRE | | 36 | | 23 | | NC | | 1.466252 | | | f1177 14 | | | f721 17 | | | f668 10 | | |
| s 38 | 1.00 | | STRE | | 36 | | 20 | | NC | | 1.474570 | | | f1106 13 | | | f897 11 | | |  | | |
| s 39 | 1.00 | | BEND | | 2 | | 3 | | 8 | | CCC | | 121.61 | | | f343 71 | | |  | | |  | |  | |
|  | 1.00 | |  | | 5 | | 4 | | 37 | | CCO | | 120.99 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 2 | | 3 | | 4 | | CCC | | 118.33 | | |  | | |  | | |  | |  | |
| s 40 | 1.00 | | BEND | | 23 | | 25 | | 29 | | CCC | | 109.95 | | | f464 29 | | |  | | |  | |  | |
|  | -1.00 | |  | | 28 | | 24 | | 39 | | CCO | | 119.45 | | |  | | |  | | |  | |  | |
| s 41 | 1.00 | | BEND | | 38 | | 37 | | 4 | | HOC | | 109.09 | | | f1202 34 | | |  | | |  | |  | |
| s 42 | 1.00 | | BEND | | 7 | | 5 | | 6 | | HCC | | 119.53 | | | f1520 11 | | | f1242 23 | | | f1202 13 | |  | |
| s 43 | 1.00 | | BEND | | 13 | | 12 | | 14 | | HCH | | 106.44 | | | f1428 81 | | |  | | |  | |  | |
|  | 1.00 | |  | | 13 | | 12 | | 15 | | HCH | | 107.68 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
| s 44 | 1.00 | | BEND | | 9 | | 8 | | 10 | | HCH | | 107.74 | | | f1520 18 | | | f1499 40 | | |  | |  | |
|  | -1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.13 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 13 | | 12 | | 14 | | HCH | | 106.44 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 107.36 | | |  | | |  | | |  | |  | |
| s 45 | 1.00 | | BEND | | 10 | | 8 | | 11 | | HCH | | 108.21 | | | f1502 59 | | |  | | |  | |  | |
|  | -1.00 | |  | | 34 | | 29 | | 35 | | HCH | | 106.67 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 106.85 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 13 | | 12 | | 15 | | HCH | | 107.68 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 30 | | 25 | | 31 | | HCH | | 107.13 | | |  | | |  | | |  | |  | |
| s 46 | 1.00 | | BEND | | 9 | | 8 | | 11 | | HCH | | 106.85 | | | f1416 67 | | |  | | |  | |  | |
|  | -1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 13 | | 12 | | 15 | | HCH | | 107.68 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.74 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 10 | | 8 | | 11 | | HCH | | 108.21 | | |  | | |  | | |  | |  | |
| s 47 | -1.00 | | BEND | | 13 | | 12 | | 15 | | HCH | | 107.68 | | | f1513 67 | | | f1040 14 | | |  | |  | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.74 | | |  | | |  | | |  | |  | |
| s 48 | 1.00 | | BEND | | 14 | | 12 | | 15 | | HCH | | 107.41 | | | f1529 14 | | | f1485 36 | | | f1102 10 | |  | |
|  | -1.00 | |  | | 13 | | 12 | | 14 | | HCH | | 106.44 | | |  | | |  | | |  | |  | |
| s 49 | 1.00 | | BEND | | 17 | | 16 | | 18 | | HCH | | 107.13 | | | f1419 92 | | |  | | |  | |  | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 107.36 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 18 | | 16 | | 19 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
| s 50 | -1.00 | | BEND | | 9 | | 8 | | 11 | | HCH | | 106.85 | | | f1488 57 | | |  | | |  | |  | |
|  | 1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.13 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 18 | | 16 | | 19 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.74 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
| s 51 | -1.00 | | BEND | | 17 | | 16 | | 19 | | HCH | | 107.36 | | | f1491 55 | | | f1485 10 | | | f1057 19 | |  | |
|  | 1.00 | |  | | 18 | | 16 | | 19 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
| s 52 | 1.00 | | BEND | | 21 | | 20 | | 1 | | HCC | | 111.50 | | | f1177 12 | | |  | | |  | |  | |
| s 53 | 1.00 | | BEND | | 22 | | 20 | | 21 | | HCH | | 106.63 | | | f1529 23 | | | f1528 13 | | | f1520 17 | | f1485 15 | |
| s 54 | 1.00 | | BEND | | 26 | | 23 | | 25 | | HCC | | 109.49 | | | f1308 36 | | | f1282 11 | | |  | |  | |
| s 55 | 1.00 | | BEND | | 27 | | 23 | | 26 | | HCH | | 107.03 | | | f1529 19 | | | f1528 47 | | |  | |  | |
| s 56 | 1.00 | | BEND | | 30 | | 25 | | 29 | | HCC | | 111.51 | | | f1363 19 | | |  | | |  | |  | |
| s 57 | 1.00 | | BEND | | 34 | | 29 | | 35 | | HCH | | 106.67 | | | f1503 51 | | |  | | |  | |  | |
|  | 1.00 | |  | | 10 | | 8 | | 11 | | HCH | | 108.21 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 106.85 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.41 | | |  | | |  | | |  | |  | |
| s 58 | 1.00 | | BEND | | 32 | | 28 | | 29 | | HCC | | 112.26 | | | f1290 29 | | | f1282 10 | | |  | |  | |
| s 59 | 1.00 | | BEND | | 33 | | 28 | | 32 | | HCH | | 106.16 | | | f1475 42 | | | f1458 34 | | |  | |  | |
| s 60 | 1.00 | | BEND | | 34 | | 29 | | 28 | | HCC | | 110.23 | | | f1355 15 | | | f1189 10 | | | f1117 14 | |  | |
| s 61 | 1.00 | | BEND | | 30 | | 25 | | 31 | | HCH | | 107.13 | | | f1493 80 | | |  | | |  | |  | |
|  | -1.00 | |  | | 34 | | 29 | | 35 | | HCH | | 106.67 | | |  | | |  | | |  | |  | |
| s 62 | 1.00 | | BEND | | 28 | | 24 | | 39 | | CCO | | 119.45 | | | f511 45 | | |  | | |  | |  | |
| s 63 | 1.00 | | BEND | | 2 | | 3 | | 4 | | CCC | | 118.33 | | | f472 22 | | | f454 10 | | |  | |  | |
| s 64 | 1.00 | | BEND | | 6 | | 5 | | 4 | | CCC | | 121.17 | | |  | | |  | | |  | |  | |
| s 65 | 1.00 | | BEND | | 1 | | 6 | | 5 | | CCC | | 119.08 | | | f1437 14 | | | f710 16 | | |  | |  | |
| s 66 | 1.00 | | BEND | | 24 | | 36 | | 20 | | CNC | | 118.66 | | | f219 28 | | |  | | |  | |  | |
| s 67 | 1.00 | | BEND | | 5 | | 6 | | 16 | | CCC | | 118.03 | | | f324 51 | | |  | | |  | |  | |
|  | -1.00 | |  | | 2 | | 3 | | 8 | | CCC | | 121.61 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 5 | | 4 | | 37 | | CCO | | 120.99 | | |  | | |  | | |  | |  | |
| s 68 | 1.00 | | BEND | | 2 | | 3 | | 4 | | CCC | | 118.33 | | | f1437 13 | | |  | | |  | |  | |
|  | 1.00 | |  | | 3 | | 4 | | 5 | | CCC | | 120.94 | | |  | | |  | | |  | |  | |
| s 69 | 1.00 | | BEND | | 3 | | 2 | | 12 | | CCC | | 117.60 | | | f593 40 | | | f579 10 | | |  | |  | |
|  | -1.00 | |  | | 5 | | 6 | | 16 | | CCC | | 118.03 | | |  | | |  | | |  | |  | |
|  | 1.00 | |  | | 5 | | 4 | | 37 | | CCO | | 120.99 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 2 | | 3 | | 8 | | CCC | | 121.61 | | |  | | |  | | |  | |  | |
| s 70 | 1.00 | | BEND | | 3 | | 2 | | 12 | | CCC | | 117.60 | | | f371 23 | | | f356 48 | | |  | |  | |
|  | 1.00 | |  | | 2 | | 3 | | 8 | | CCC | | 121.61 | | |  | | |  | | |  | |  | |
| s 71 | 1.00 | | BEND | | 20 | | 1 | | 2 | | CCC | | 120.48 | | | f396 34 | | | f219 19 | | |  | |  | |
| s 72 | 1.00 | | BEND | | 23 | | 25 | | 29 | | CCC | | 109.95 | | | f996 10 | | | f976 10 | | | f464 12 | |  | |
|  | 1.00 | |  | | 25 | | 23 | | 36 | | CCN | | 113.25 | | |  | | |  | | |  | |  | |
|  | -1.00 | |  | | 28 | | 24 | | 39 | | CCO | | 119.45 | | |  | | |  | | |  | |  | |
| s 73 | 1.00 | | BEND | | 28 | | 24 | | 36 | | CCN | | 118.11 | | | f668 11 | | |  | | |  | |  | |
| s 74 | 1.00 | | BEND | | 23 | | 36 | | 24 | | CNC | | 123.86 | | |  | | |  | | |  | |  | |
| s 75 | 1.00 | | BEND | | 36 | | 20 | | 1 | | NCC | | 114.15 | | | f548 12 | | | f45 19 | | |  | |  | |
| s 76 | 1.00 | | TORS | | 38 | | 37 | | 4 | | 5 | | HOCC | | | -0.22 | | | f322 15 | | | f313 61 | | f289 11 | |
| s 77 | 1.00 | | TORS | | 7 | | 5 | | 6 | | 16 | | HCCC | | | -0.54 | | | f841 62 | | |  | |  | |
| s 78 | 1.00 | | TORS | | 9 | | 8 | | 3 | | 4 | | HCCC | | | -247.16 | | | f114 12 | | |  | |  | |
| s 79 | 1.00 | | TORS | | 10 | | 8 | | 3 | | 4 | | HCCC | | | -7.27 | | | f1073 23 | | | f1070 20 | | f110 14 | |
|  | 1.00 | |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -11.12 | | |  | | |  | |  | |
| s 80 | 1.00 | | TORS | | 11 | | 8 | | 3 | | 4 | | HCCC | | | -127.94 | | |  | | |  | |  | |
| s 81 | 1.00 | | TORS | | 13 | | 12 | | 2 | | 1 | | HCCC | | | -132.22 | | | f1102 12 | | | f178 10 | |  | |
| s 82 | 1.00 | | TORS | | 14 | | 12 | | 2 | | 1 | | HCCC | | | -250.13 | | | f1102 15 | | | f178 15 | |  | |
| s 83 | -1.00 | | TORS | | 10 | | 8 | | 3 | | 4 | | HCCC | | | -7.27 | | | f1040 60 | | |  | |  | |
|  | 1.00 | |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -11.12 | | |  | | |  | |  | |
| s 84 | 1.00 | | TORS | | 17 | | 16 | | 6 | | 5 | | HCCC | | | -116.94 | | | f170 58 | | |  | |  | |
|  | 1.00 | |  | | 18 | | 16 | | 6 | | 5 | | HCCC | | | -237.57 | | |  | | |  | |  | |
| s 85 | -1.00 | | TORS | | 17 | | 16 | | 6 | | 5 | | HCCC | | | -116.94 | | | f1053 29 | | | f1025 21 | |  | |
|  | 1.00 | |  | | 18 | | 16 | | 6 | | 5 | | HCCC | | | -237.57 | | |  | | |  | |  | |
| s 86 | 1.00 | | TORS | | 19 | | 16 | | 6 | | 5 | | HCCC | | | 2.58 | | | f1057 53 | | |  | |  | |
| s 87 | -1.00 | | TORS | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -128.84 | | | f1386 49 | | |  | |  | |
|  | 1.00 | |  | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -10.75 | | |  | | |  | |  | |
|  | 1.00 | |  | | 31 | | 25 | | 29 | | 28 | | HCCC | | | 61.21 | | |  | | |  | |  | |
| s 88 | 1.00 | | TORS | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -128.84 | | | f897 16 | | |  | |  | |
|  | 1.00 | |  | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -10.75 | | |  | | |  | |  | |
| s 89 | 1.00 | | TORS | | 26 | | 23 | | 36 | | 20 | | HCNC | | | -70.41 | | | f1117 10 | | |  | |  | |
| s 90 | 1.00 | | TORS | | 27 | | 23 | | 36 | | 20 | | HCNC | | | 45.34 | | | f1475 11 | | | f1458 14 | |  | |
| s 91 | 1.00 | | TORS | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -128.84 | | | f1389 58 | | |  | |  | |
|  | -1.00 | |  | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -10.75 | | |  | | |  | |  | |
|  | -1.00 | |  | | 30 | | 25 | | 29 | | 28 | | HCCC | | | -180.18 | | |  | | |  | |  | |
|  | 1.00 | |  | | 31 | | 25 | | 29 | | 28 | | HCCC | | | 61.21 | | |  | | |  | |  | |
| s 92 | 1.00 | | TORS | | 30 | | 25 | | 29 | | 28 | | HCCC | | | -180.18 | | | f322 16 | | |  | |  | |
|  | 1.00 | |  | | 31 | | 25 | | 29 | | 28 | | HCCC | | | 61.21 | | |  | | |  | |  | |
| s 93 | 1.00 | | TORS | | 32 | | 28 | | 24 | | 36 | | HCCN | | | -146.80 | | | f1290 10 | | | f568 14 | |  | |
| s 94 | 1.00 | | TORS | | 33 | | 28 | | 24 | | 36 | | HCCN | | | -259.35 | | | f1355 20 | | | f1282 11 | |  | |
| s 95 | 1.00 | | TORS | | 31 | | 25 | | 29 | | 28 | | HCCC | | | 61.21 | | | f1380 38 | | |  | |  | |
|  | 1.00 | |  | | 34 | | 29 | | 28 | | 24 | | HCCC | | | -192.12 | | |  | | |  | |  | |
|  | -1.00 | |  | | 35 | | 29 | | 28 | | 24 | | HCCC | | | -74.75 | | |  | | |  | |  | |
| s 96 | 1.00 | | TORS | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -128.84 | | | f942 10 | | |  | |  | |
|  | 1.00 | |  | | 30 | | 25 | | 29 | | 28 | | HCCC | | | -180.18 | | |  | | |  | |  | |
|  | -1.00 | |  | | 31 | | 25 | | 29 | | 28 | | HCCC | | | 61.21 | | |  | | |  | |  | |
|  | 1.00 | |  | | 34 | | 29 | | 28 | | 24 | | HCCC | | | -192.12 | | |  | | |  | |  | |
|  | 1.00 | |  | | 35 | | 29 | | 28 | | 24 | | HCCC | | | -74.75 | | |  | | |  | |  | |
| s 97 | -1.00 | | TORS | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.01 | | | f97 47 | | |  | |  | |
|  | 1.00 | |  | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.63 | | |  | | |  | |  | |
|  | -1.00 | |  | | 20 | | 36 | | 23 | | 25 | | CNCC | | | -192.61 | | |  | | |  | |  | |
|  | 1.00 | |  | | 20 | | 36 | | 24 | | 28 | | CNCC | | | -182.92 | | |  | | |  | |  | |
| s 98 | 1.00 | | OUT | | 8 | | 2 | | 4 | | 3 | | CCCC | | | 0.28 | | | f772 23 | | | f721 11 | |  | |
|  | -1.00 | |  | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.72 | | |  | | |  | |  | |
|  | 1.00 | | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | 1.00 | |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.01 | | |  | | |  | |  | |
|  | -1.00 | | OUT | | 37 | | 3 | | 5 | | 4 | | OCCC | | | 0.28 | | |  | | |  | |  | |
| s 99 | 1.00 | | TORS | | 1 | | 20 | | 36 | | 24 | | CCNC | | | -228.36 | | | f45 46 | | |  | |  | |
|  | 1.00 | |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.01 | | |  | | |  | |  | |
|  | 1.00 | |  | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.63 | | |  | | |  | |  | |
|  | 1.00 | |  | | 6 | | 1 | | 20 | | 36 | | CCCN | | | -249.03 | | |  | | |  | |  | |
| s 100 | 1.00 | | TORS | | 1 | | 20 | | 36 | | 24 | | CCNC | | | -228.36 | | | f57 67 | | |  | |  | |
|  | -1.00 | |  | | 6 | | 1 | | 20 | | 36 | | CCCN | | | -249.03 | | |  | | |  | |  | |
| s 101 | 1.00 | | OUT | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.72 | | | f37 57 | | |  | |  | |
|  | 1.00 | | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | -1.00 | |  | | 1 | | 20 | | 36 | | 24 | | CCNC | | | -228.36 | | |  | | |  | |  | |
|  | 1.00 | |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.01 | | |  | | |  | |  | |
|  | 1.00 | |  | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.63 | | |  | | |  | |  | |
|  | -1.00 | |  | | 6 | | 1 | | 20 | | 36 | | CCCN | | | -249.03 | | |  | | |  | |  | |
|  | 1.00 | |  | | 20 | | 36 | | 23 | | 25 | | CNCC | | | -192.61 | | |  | | |  | |  | |
|  | -1.00 | | OUT | | 37 | | 3 | | 5 | | 4 | | OCCC | | | 0.28 | | |  | | |  | |  | |
| s 102 | 1.00 | | TORS | | 20 | | 36 | | 23 | | 25 | | CNCC | | | -192.61 | | | f942 16 | | | f114 34 | |  | |
|  | 1.00 | |  | | 20 | | 36 | | 24 | | 28 | | CNCC | | | -182.92 | | |  | | |  | |  | |
| s 103 | 1.00 | | TORS | | 29 | | 25 | | 23 | | 36 | | CCCN | | | 50.62 | | | f1117 19 | | | f322 15 | |  | |
| s 104 | 1.00 | | OUT | | 8 | | 2 | | 4 | | 3 | | CCCC | | | 0.28 | | | f255 34 | | |  | |  | |
|  | 1.00 | |  | | 23 | | 20 | | 24 | | 36 | | CCCN | | | 12.33 | | |  | | |  | |  | |
|  | -1.00 | | TORS | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.63 | | |  | | |  | |  | |
| s 105 | 1.00 | | OUT | | 39 | | 28 | | 36 | | 24 | | OCNC | | | 2.65 | | | f668 17 | | | f643 12 | | f568 16 | |
| s 106 | -1.00 | | OUT | | 16 | | 1 | | 5 | | 6 | | CCCC | | | 0.67 | | | f211 44 | | | f170 10 | |  | |
|  | 1.00 | | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | 1.00 | | OUT | | 37 | | 3 | | 5 | | 4 | | OCCC | | | 0.28 | | |  | | |  | |  | |
| s 107 | 1.00 | | OUT | | 16 | | 1 | | 5 | | 6 | | CCCC | | | 0.67 | | | f643 13 | | | f548 18 | |  | |
| s 108 | 1.00 | | OUT | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.17 | | | f553 63 | | |  | |  | |
|  | 1.00 | |  | | 16 | | 1 | | 5 | | 6 | | CCCC | | | 0.67 | | |  | | |  | |  | |
|  | -1.00 | |  | | 37 | | 3 | | 5 | | 4 | | OCCC | | | 0.28 | | |  | | |  | |  | |
| s 109 | -1.00 | | OUT | | 8 | | 2 | | 4 | | 3 | | CCCC | | | 0.28 | | | f289 54 | | |  | |  | |
|  | -1.00 | |  | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | -1.00 | |  | | 16 | | 1 | | 5 | | 6 | | CCCC | | | 0.67 | | |  | | |  | |  | |
|  | 1.00 | | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.17 | | |  | | |  | |  | |
| s 110 | -1.00 | | OUT | | 8 | | 2 | | 4 | | 3 | | CCCC | | | 0.28 | | | f371 11 | | | f178 10 | | f141 24 | |
|  | -1.00 | |  | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.72 | | |  | | |  | |  | |
|  | 1.00 | |  | | 23 | | 20 | | 24 | | 36 | | CCCN | | | 12.33 | | |  | | |  | |  | |
|  | 1.00 | | TORS | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.63 | | |  | | |  | |  | |
|  | 1.00 | |  | | 20 | | 36 | | 23 | | 25 | | CNCC | | | -192.61 | | |  | | |  | |  | |
| s 111 | 1.00 | | OUT | | 8 | | 2 | | 4 | | 3 | | CCCC | | | 0.28 | | | f125 39 | | | f110 23 | |  | |
|  | -1.00 | |  | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | -1.00 | |  | | 16 | | 1 | | 5 | | 6 | | CCCC | | | 0.67 | | |  | | |  | |  | |
|  | -1.00 | |  | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.72 | | |  | | |  | |  | |
|  | 1.00 | | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.17 | | |  | | |  | |  | |
|  | -1.00 | |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.01 | | |  | | |  | |  | |
|  | 1.00 | |  | | 20 | | 36 | | 23 | | 25 | | CNCC | | | -192.61 | | |  | | |  | |  | |

Experimental and calculated wavenumbers of FT-IR spectra of compound 8 by DFT/B3LYP method.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| IR observed ν(cm-1) | IR calculated, scaled ν(cm-1) | IR calculated, unscaled ν(cm-1 | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % | Vibration | PED, % |
| 3443 | 3683,73 | 3832,03 | s1 | 100 |  |  |  |  |  |  |
| 3030 | 3015,896 | 3137,31 | s2 | 95 |  |  |  |  |  |  |
| 3022 | 3013,493 | 3134,81 | s11 | 86 |  |  |  |  |  |  |
| - | 2997,891 | 3118,58 | s7 | -90 |  |  |  |  |  |  |
| - | 2991,402 | 3111,83 | s18 | -87 |  |  |  |  |  |  |
| - | 2988,057 | 3108,35 | s14 | 76 | s15 | -20 |  |  |  |  |
| 2972 | 2978,761 | 3098,68 | s3 | 79 | s5 | -18 |  |  |  |  |
| 2970 | 2976,175 | 3095,99 | s6 | 89 |  |  |  |  |  |  |
| 2955 | 2960,4 | 3079,58 | s12 | 79 |  |  |  |  |  |  |
| 2950 | 2954,652 | 3073,6 | s4 | 96 |  |  |  |  |  |  |
| 2945 | 2951,604 | 3070,43 | s9 | -90 |  |  |  |  |  |  |
| 2941 | 2946,606 | 3065,23 | s19 | 83 |  |  |  |  |  |  |
| - | 2944,212 | 3062,74 | s20 | 68 |  |  |  |  |  |  |
| 2930 | 2941,049 | 3059,45 | s14 | 15 | s15 | 66 |  |  |  |  |
| - | 2939,8 | 3058,15 | s22 | -81 |  |  |  |  |  |  |
| - | 2925,572 | 3043,35 | s16 | 79 |  |  |  |  |  |  |
| 2916 | 2923,409 | 3041,1 | s8 | 15 | s13 | 61 |  |  |  |  |
| - | 2922,439 | 3040,09 | s8 | 79 | s13 | -13 |  |  |  |  |
| 2892 | 2912,297 | 3029,54 | s23 | 85 |  |  |  |  |  |  |
| 2858 | 2908,913 | 3026,02 | s3 | 15 | s5 | 77 |  |  |  |  |
| 2952 | 2905,837 | 3022,82 | s21 | 83 |  |  |  |  |  |  |
| - | 2905,52 | 3022,49 | s10 | 85 |  |  |  |  |  |  |
| 2835 | 2896,262 | 3012,86 | s17 | 91 |  |  |  |  |  |  |
| 1620 | 1667,932 | 1735,08 | s24 | 88 |  |  |  |  |  |  |
| 1599 | 1573,6 | 1636,95 | s25 | 48 | s42 | 12 |  |  |  |  |
| 1572 | 1561,17 | 1624,02 | s27 | -10 | s28 | 54 |  |  |  |  |
| 1491 | 1463,56 | 1522,48 | s29 | 30 | s45 | -15 | s50 | 12 |  |  |
| 1485 | 1462,272 | 1521,14 | s51 | 65 |  |  |  |  |  |  |
| 1471 | 1450,525 | 1508,92 | s56 | -53 |  |  |  |  |  |  |
| 1462 | 1445,478 | 1503,67 | s49 | 54 |  |  |  |  |  |  |
| 1458 | 1444,353 | 1502,5 | s66 | 53 |  |  |  |  |  |  |
| 1454 | 1443,642 | 1501,76 | s47 | -48 |  |  |  |  |  |  |
| 1442 | 1441,517 | 1499,55 | s58 | 77 |  |  |  |  |  |  |
| 1437 | 1434,163 | 1491,9 | s53 | -69 |  |  |  |  |  |  |
| - | 1431,731 | 1489,37 | s64 | -77 |  |  |  |  |  |  |
| - | 1428,405 | 1485,91 | s46 | 59 |  |  |  |  |  |  |
| 1425 | 1425,56 | 1482,95 | s60 | 56 |  |  |  |  |  |  |
| - | 1423,993 | 1481,32 | s62 | 73 |  |  |  |  |  |  |
| 1408 | 1416,235 | 1473,25 | s50 | -55 |  |  |  |  |  |  |
| 1383 | 1380,484 | 1436,06 |  |  |  |  |  |  |  |  |
| - | 1367,478 | 1422,53 | s48 | 11 | s54 | 67 |  |  |  |  |
| - | 1363,873 | 1418,78 | s48 | 73 |  |  |  |  |  |  |
| - | 1360,143 | 1414,9 | s52 | 75 |  |  |  |  |  |  |
| 1352 | 1341,119 | 1395,11 | s57 | 23 | s93 | -15 | s96 | 11 |  |  |
| 1346 | 1337,207 | 1391,04 | s93 | 30 | s102 | 14 |  |  |  |  |
| - | 1328,757 | 1382,25 | s95 | 51 |  |  |  |  |  |  |
| 1334 | 1325,296 | 1378,65 | s59 | 20 | s65 | 11 | s96 | -10 |  |  |
| - | 1320,769 | 1373,94 | s63 | 11 | s102 | -14 | s104 | 13 |  |  |
| 1315 | 1311,55 | 1364,35 | s55 | 11 | s57 | -16 |  |  |  |  |
| 1290 | 1281,038 | 1332,61 | s61 | 13 | s65 | 19 | s104 | -15 |  |  |
| - | 1273,953 | 1325,24 | s26 | 41 |  |  |  |  |  |  |
| 1280 | 1271,656 | 1322,85 | s27 | -13 | s31 | 23 | s32 | 11 | s33 | 11 |
| 1246 | 1245,403 | 1295,54 | s44 | 10 | s55 | -11 | s57 | -10 |  |  |
| 1228 | 1229,772 | 1279,28 | s59 | -18 | s61 | -11 | s65 | 12 | s100 | 17 |
| - | 1221,687 | 1270,87 | s45 | 18 |  |  |  |  |  |  |
| 1207 | 1210,344 | 1259,07 | s61 | 13 | s63 | 18 |  |  |  |  |
| 1193 | 1198,933 | 1247,2 | s34 | 11 | s35 | 10 | s43 | 10 |  |  |
| 1176 | 1186,734 | 1234,51 | s45 | -18 |  |  |  |  |  |  |
| 1147 | 1162,135 | 1208,92 | s65 | -11 | s98 | 37 | s100 | -11 |  |  |
| 1145 | 1152,781 | 1199,19 | s26 | -10 | s44 | 36 | s45 | -17 |  |  |
| 1138 | 1137,766 | 1183,57 | s38 | -10 |  |  |  |  |  |  |
| - | 1085,404 | 1129,1 | s113 | -10 |  |  |  |  |  |  |
| 1097 | 1060,948 | 1103,66 | s37 | 18 |  |  |  |  |  |  |
| 1095 | 1055,623 | 1098,12 | s31 | -11 | s92 | -35 |  |  |  |  |
| 1085 | 1049,547 | 1091,8 | s31 | 16 | s34 | -13 | s35 | 13 |  |  |
| 1053 | 1027,659 | 1069,03 | s90 | 50 |  |  |  |  |  |  |
| - | 1024,477 | 1065,72 | s40 | -47 |  |  |  |  |  |  |
| 1028 | 1016,709 | 1057,64 | s84 | -36 |  |  |  |  |  |  |
| - | 1015,056 | 1055,92 | s85 | -48 |  |  |  |  |  |  |
| 997 | 997,3776 | 1037,53 | s88 | -48 |  |  |  |  |  |  |
| 974 | 986,8514 | 1026,58 | s85 | 10 | s91 | 32 |  |  |  |  |
| 960 | 974,5852 | 1013,82 | s39 | 26 | s81 | 11 | s103 | 10 |  |  |
| - | 961,5403 | 1000,25 | s36 | -10 | s94 | 11 | s113 | -11 |  |  |
| 941 | 936,6619 | 974,37 | s94 | -13 |  |  |  |  |  |  |
| - | 926,972 | 964,29 | s30 | -10 |  |  |  |  |  |  |
| 908 | 920,1467 | 957,19 |  |  |  |  |  |  |  |  |
| 879 | 883,4443 | 919,01 | s33 | 13 | s69 | 13 |  |  |  |  |
| 864 | 835,562 | 869,2 | s80 | 11 |  |  |  |  |  |  |
| 860 | 825,0165 | 858,23 | s79 | -11 | s109 | -10 |  |  |  |  |
| 850 | 815,8745 | 848,72 | s35 | -11 |  |  |  |  |  |  |
| 835 | 807,4343 | 839,94 | s83 | -61 | s115 | -19 |  |  |  |  |
| 812 | 783,248 | 814,78 | s97 | -13 |  |  |  |  |  |  |
| 759 | 756,6681 | 787,13 | s30 | 11 | s36 | 12 |  |  |  |  |
| 740 | 727,8098 | 757,11 | s39 | 15 | s41 | 26 | s115 | 11 |  |  |
| 709 | 702,816 | 731,11 | s38 | 11 |  |  |  |  |  |  |
| 694 | 689,1079 | 716,85 | s99 | 10 | s114 | -10 |  |  |  |  |
| 682 | 680,5139 | 707,91 | s34 | -12 |  |  |  |  |  |  |
| - | 625,5371 | 650,72 | s117 | -28 |  |  |  |  |  |  |
|  | 582,3363 | 605,78 | s67 | 18 | s74 | -12 | s117 | -11 |  |  |
| 12 | 557,1695 | 579,6 | s27 | 11 | s31 | 11 | s32 | 10 | s33 | 13 |
|  | 552,1803 | 574,41 | s72 | -10 | s73 | 11 | s74 | 20 |  |  |
|  | 527,4269 | 548,66 | s106 | -57 |  |  |  |  |  |  |
|  | 525,6869 | 546,85 | s33 | -10 | s68 | -12 |  |  |  |  |
|  | 494,8196 | 514,74 | s79 | 20 | s81 | 10 | s101 | 29 |  |  |
|  | 454,8968 | 473,21 | s43 | 11 | s68 | 13 | s69 | 11 |  |  |
|  | 438,2951 | 455,94 | s70 | 35 |  |  |  |  |  |  |
|  | 406,1781 | 422,53 | s81 | 15 |  |  |  |  |  |  |
|  | 380,646 | 395,97 | s116 | 10 | s117 | -17 | s120 | -13 |  |  |
|  | 372,8787 | 387,89 | s73 | 29 |  |  |  |  |  |  |
|  | 353,7392 | 367,98 | s73 | 10 |  |  |  |  |  |  |
|  | 332,3599 | 345,74 | s71 | 70 |  |  |  |  |  |  |
|  | 331,2928 | 344,63 |  |  |  |  |  |  |  |  |
|  | 319,4592 | 332,32 | s72 | 24 |  |  |  |  |  |  |
|  | 303,5209 | 315,74 | s72 | 26 | s74 | 17 |  |  |  |  |
|  | 295,3883 | 307,28 | s82 | 51 |  |  |  |  |  |  |
|  | 280,1036 | 291,38 | s82 | 17 |  |  |  |  |  |  |
|  | 274,4127 | 285,46 | s82 | 15 | s115 | 10 | s116 | -18 |  |  |
|  | 201,0174 | 209,11 | s86 | 11 | s107 | 56 |  |  |  |  |
|  | 196,1917 | 204,09 | s35 | 10 | s77 | 39 |  |  |  |  |
|  | 169,631 | 176,46 | s107 | -12 | s111 | 22 |  |  |  |  |
|  | 153,9714 | 160,17 | s86 | 55 |  |  |  |  |  |  |
|  | 149,4822 | 155,5 | s86 | 19 | s87 | -16 | s120 | 16 |  |  |
|  | 130,5926 | 135,85 | s87 | 30 | s109 | -11 |  |  |  |  |
|  | 116,0001 | 120,67 | s87 | 11 | s109 | 17 | s114 | -14 | s120 | 10 |
|  | 105,9064 | 110,17 | s105 | -60 |  |  |  |  |  |  |
|  | 101,3114 | 105,39 | s89 | 12 | s112 | 43 |  |  |  |  |
|  | 94,84186 | 98,66 | s89 | 71 |  |  |  |  |  |  |
|  | 55,48624 | 57,72 | s108 | -71 |  |  |  |  |  |  |
|  | 46,56537 | 48,44 | s76 | -23 | s118 | 52 |  |  |  |  |
|  | 18,87993 | 19,64 | \* | 18.97 | s110 | 80 |  |  |  |  |

Scaling factor = 0.9613, (-)PED% - asymmetric vibrations

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| s 1 | 1.00 | | STRE | | 39 | | 40 | | OH | | 0.963461 | | | f3832 100 | | |  | | |  | | |  | | |
| s 2 | 1.00 | | STRE | | 5 | | 7 | | CH | | 1.086402 | | | f3137 95 | | |  | | |  | | |  | | |
| s 3 | 1.00 | | STRE | | 8 | | 9 | | CH | | 1.090609 | | | f3099 79 | | | f3026 15 | | |  | | |  | | |
| s 4 | 1.00 | | STRE | | 8 | | 10 | | CH | | 1.093314 | | | f3074 96 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 8 | | 11 | | CH | | 1.092483 | | |  | | |  | | |  | | |  | | |
| s 5 | 1.00 | | STRE | | 8 | | 10 | | CH | | 1.093314 | | | f3099 18 | | | f3026 77 | | |  | | |  | | |
|  | 1.00 | |  | | 8 | | 11 | | CH | | 1.092483 | | |  | | |  | | |  | | |  | | |
| s 6 | 1.00 | | STRE | | 12 | | 13 | | CH | | 1.093411 | | | f3096 89 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 12 | | 15 | | CH | | 1.089128 | | |  | | |  | | |  | | |  | | |
| s 7 | -1.00 | | STRE | | 12 | | 14 | | CH | | 1.089323 | | | f3119 90 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 12 | | 15 | | CH | | 1.089128 | | |  | | |  | | |  | | |  | | |
| s 8 | 1.00 | | STRE | | 12 | | 13 | | CH | | 1.093411 | | | f3041 15 | | | f3040 79 | | |  | | |  | | |
|  | 1.00 | |  | | 12 | | 14 | | CH | | 1.089323 | | |  | | |  | | |  | | |  | | |
| s 9 | 1.00 | | STRE | | 16 | | 17 | | CH | | 1.092152 | | | f3070 90 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 16 | | 18 | | CH | | 1.094722 | | |  | | |  | | |  | | |  | | |
| s 10 | 1.00 | | STRE | | 16 | | 17 | | CH | | 1.092152 | | | f3023 85 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 16 | | 18 | | CH | | 1.094722 | | |  | | |  | | |  | | |  | | |
| s 11 | 1.00 | | STRE | | 16 | | 19 | | CH | | 1.087446 | | | f3135 86 | | |  | | |  | | |  | | |
| s 12 | 1.00 | | STRE | | 20 | | 21 | | CH | | 1.092253 | | | f3080 79 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 20 | | 22 | | CH | | 1.090735 | | |  | | |  | | |  | | |  | | |
| s 13 | 1.00 | | STRE | | 25 | | 31 | | CH | | 1.095293 | | | f3041 61 | | | f3040 13 | | |  | | |  | | |
|  | -1.00 | |  | | 25 | | 30 | | CH | | 1.095400 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 20 | | 21 | | CH | | 1.092253 | | |  | | |  | | |  | | |  | | |
| s 14 | 1.00 | | STRE | | 23 | | 26 | | CH | | 1.089431 | | | f3108 76 | | | f3059 15 | | |  | | |  | | |
| s 15 | 1.00 | | STRE | | 23 | | 27 | | CH | | 1.091788 | | | f3108 20 | | | f3059 66 | | |  | | |  | | |
| s 16 | 1.00 | | STRE | | 20 | | 21 | | CH | | 1.092253 | | | f3043 79 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 20 | | 22 | | CH | | 1.090735 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 25 | | 30 | | CH | | 1.095400 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 25 | | 31 | | CH | | 1.095293 | | |  | | |  | | |  | | |  | | |
| s 17 | 1.00 | | STRE | | 25 | | 30 | | CH | | 1.095400 | | | f3013 91 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 25 | | 31 | | CH | | 1.095293 | | |  | | |  | | |  | | |  | | |
| s 18 | 1.00 | | STRE | | 28 | | 33 | | CH | | 1.089142 | | | f3112 87 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 28 | | 34 | | CH | | 1.091178 | | |  | | |  | | |  | | |  | | |
| s 19 | -1.00 | | STRE | | 29 | | 35 | | CH | | 1.094398 | | | f3065 83 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 29 | | 36 | | CH | | 1.093808 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 32 | | 37 | | CH | | 1.092495 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 32 | | 38 | | CH | | 1.093338 | | |  | | |  | | |  | | |  | | |
| s 20 | 1.00 | | STRE | | 28 | | 34 | | CH | | 1.091178 | | | f3063 68 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 32 | | 37 | | CH | | 1.092495 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 28 | | 33 | | CH | | 1.089142 | | |  | | |  | | |  | | |  | | |
| s 21 | 1.00 | | STRE | | 29 | | 35 | | CH | | 1.094398 | | | f3023 83 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 29 | | 36 | | CH | | 1.093808 | | |  | | |  | | |  | | |  | | |
| s 22 | -1.00 | | STRE | | 28 | | 33 | | CH | | 1.089142 | | | f3058 81 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 28 | | 34 | | CH | | 1.091178 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 29 | | 35 | | CH | | 1.094398 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 29 | | 36 | | CH | | 1.093808 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 32 | | 37 | | CH | | 1.092495 | | |  | | |  | | |  | | |  | | |
| s 23 | 1.00 | | STRE | | 32 | | 37 | | CH | | 1.092495 | | | f3030 85 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 32 | | 38 | | CH | | 1.093338 | | |  | | |  | | |  | | |  | | |
| s 24 | 1.00 | | STRE | | 41 | | 24 | | OC | | 1.214771 | | | f1735 88 | | |  | | |  | | |  | | |
| s 25 | 1.00 | | STRE | | 4 | | 5 | | CC | | 1.387511 | | | f1637 48 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 2 | | 3 | | CC | | 1.404537 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 3 | | 4 | | CC | | 1.396454 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 1 | | 6 | | CC | | 1.404480 | | |  | | |  | | |  | | |  | | |
| s 26 | 1.00 | | STRE | | 2 | | 3 | | CC | | 1.404537 | | | f1325 41 | | | f1199 10 | | |  | | |  | | |
|  | 1.00 | |  | | 1 | | 6 | | CC | | 1.404480 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 4 | | 5 | | CC | | 1.387511 | | |  | | |  | | |  | | |  | | |
| s 27 | 1.00 | | STRE | | 4 | | 5 | | CC | | 1.387511 | | | f1624 10 | | | f1323 13 | | | f580 11 | | |  | | |
|  | 1.00 | |  | | 5 | | 6 | | CC | | 1.391566 | | |  | | |  | | |  | | |  | | |
| s 28 | -1.00 | | STRE | | 5 | | 6 | | CC | | 1.391566 | | | f1624 54 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 4 | | CC | | 1.396454 | | |  | | |  | | |  | | |  | | |
| s 29 | -1.00 | | STRE | | 1 | | 6 | | CC | | 1.404480 | | | f1522 30 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 2 | | 3 | | CC | | 1.404537 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 3 | | 4 | | CC | | 1.396454 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 4 | | 5 | | CC | | 1.387511 | | |  | | |  | | |  | | |  | | |
| s 30 | 1.00 | | STRE | | 42 | | 24 | | NC | | 1.404843 | | | f964 10 | | | f787 11 | | |  | | |  | | |
| s 31 | 1.00 | | STRE | | 39 | | 4 | | OC | | 1.374814 | | | f1323 23 | | | f1098 11 | | | f1092 16 | | | f580 11 | | |
| s 32 | 1.00 | | STRE | | 8 | | 6 | | CC | | 1.513441 | | | f1323 11 | | | f580 10 | | |  | | |  | | |
| s 33 | 1.00 | | STRE | | 12 | | 2 | | CC | | 1.511426 | | | f1323 11 | | | f919 13 | | | f580 13 | | | f547 10 | | |
| s 34 | 1.00 | | STRE | | 16 | | 3 | | CC | | 1.510057 | | | f1247 11 | | | f1092 13 | | | f708 12 | | |  | | |
| s 35 | 1.00 | | STRE | | 20 | | 1 | | CC | | 1.520315 | | | f1247 10 | | | f1092 13 | | | f849 11 | | | f204 10 | | |
| s 36 | 1.00 | | STRE | | 28 | | 24 | | CC | | 1.516561 | | | f1000 10 | | | f787 12 | | |  | | |  | | |
| s 37 | 1.00 | | STRE | | 42 | | 20 | | NC | | 1.471949 | | | f1104 18 | | |  | | |  | | |  | | |
| s 38 | 1.00 | | STRE | | 42 | | 23 | | NC | | 1.472414 | | | f1184 10 | | | f731 11 | | |  | | |  | | |
| s 39 | 1.00 | | STRE | | 25 | | 23 | | CC | | 1.542384 | | | f1014 26 | | | f757 15 | | |  | | |  | | |
| s 40 | -1.00 | | STRE | | 29 | | 32 | | CC | | 1.549593 | | | f1066 47 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 25 | | 29 | | CC | | 1.546995 | | |  | | |  | | |  | | |  | | |
| s 41 | 1.00 | | STRE | | 25 | | 29 | | CC | | 1.546995 | | | f757 26 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 29 | | 32 | | CC | | 1.549593 | | |  | | |  | | |  | | |  | | |
| s 42 | 1.00 | | BEND | | 2 | | 3 | | 4 | | CCC | | 118.18 | | | f1637 12 | | | f1323 11 | | | f580 12 | | |  | | |
| s 43 | -1.00 | | BEND | | 1 | | 6 | | 5 | | CCC | | 118.95 | | | f1247 10 | | | f473 11 | | |  | | |  | | |
|  | 1.00 | |  | | 28 | | 24 | | 41 | | CCO | | 120.91 | | |  | | |  | | |  | | |  | | |
| s 44 | 1.00 | | BEND | | 40 | | 39 | | 4 | | HOC | | 109.09 | | | f1296 10 | | | f1199 36 | | |  | | |  | | |
| s 45 | 1.00 | | BEND | | 7 | | 5 | | 4 | | HCC | | 119.30 | | | f1522 15 | | | f1271 18 | | | f1235 18 | | | f1199 17 | | |
| s 46 | -1.00 | | BEND | | 30 | | 25 | | 31 | | HCH | | 105.73 | | | f1486 59 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 107.28 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 26 | | 23 | | 27 | | HCH | | 107.42 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.17 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 108.13 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.37 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 37 | | 32 | | 38 | | HCH | | 105.93 | | |  | | |  | | |  | | |  | | |
| s 47 | -1.00 | | BEND | | 37 | | 32 | | 38 | | HCH | | 105.93 | | | f1502 48 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 108.13 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.17 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 26 | | 23 | | 27 | | HCH | | 107.42 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 21 | | 20 | | 22 | | HCH | | 106.29 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 33 | | 28 | | 34 | | HCH | | 107.89 | | |  | | |  | | |  | | |  | | |
| s 48 | 1.00 | | BEND | | 10 | | 8 | | 11 | | HCH | | 107.30 | | | f1423 11 | | | f1419 73 | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 107.28 | | |  | | |  | | |  | | |  | | |
| s 49 | -1.00 | | BEND | | 18 | | 16 | | 19 | | HCH | | 107.52 | | | f1504 54 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 108.13 | | |  | | |  | | |  | | |  | | |
| s 50 | -1.00 | | BEND | | 13 | | 12 | | 15 | | HCH | | 107.89 | | | f1522 12 | | | f1473 55 | | |  | | |  | | |
|  | 1.00 | |  | | 13 | | 12 | | 14 | | HCH | | 106.49 | | |  | | |  | | |  | | |  | | |
| s 51 | 1.00 | | BEND | | 21 | | 20 | | 22 | | HCH | | 106.29 | | | f1521 65 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.37 | | |  | | |  | | |  | | |  | | |
| s 52 | -1.00 | | BEND | | 13 | | 12 | | 14 | | HCH | | 106.49 | | | f1415 75 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 13 | | 12 | | 15 | | HCH | | 107.89 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.17 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 108.13 | | |  | | |  | | |  | | |  | | |
| s 53 | 1.00 | | BEND | | 35 | | 29 | | 36 | | HCH | | 106.01 | | | f1492 69 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 107.28 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 26 | | 23 | | 27 | | HCH | | 107.42 | | |  | | |  | | |  | | |  | | |
| s 54 | 1.00 | | BEND | | 13 | | 12 | | 14 | | HCH | | 106.49 | | | f1423 67 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 13 | | 12 | | 15 | | HCH | | 107.89 | | |  | | |  | | |  | | |  | | |
| s 55 | 1.00 | | BEND | | 21 | | 20 | | 1 | | HCC | | 109.69 | | | f1364 11 | | | f1296 11 | | |  | | |  | | |
| s 56 | -1.00 | | BEND | | 14 | | 12 | | 15 | | HCH | | 107.37 | | | f1509 53 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 21 | | 20 | | 22 | | HCH | | 106.29 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 10 | | 8 | | 11 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
| s 57 | 1.00 | | BEND | | 26 | | 23 | | 25 | | HCC | | 110.40 | | | f1395 23 | | | f1364 16 | | | f1296 10 | | |  | | |
| s 58 | 1.00 | | BEND | | 26 | | 23 | | 27 | | HCH | | 107.42 | | | f1500 77 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 35 | | 29 | | 36 | | HCH | | 106.01 | | |  | | |  | | |  | | |  | | |
| s 59 | 1.00 | | BEND | | 30 | | 25 | | 29 | | HCC | | 108.16 | | | f1379 20 | | | f1279 18 | | |  | | |  | | |
| s 60 | 1.00 | | BEND | | 30 | | 25 | | 31 | | HCH | | 105.73 | | | f1483 56 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 21 | | 20 | | 22 | | HCH | | 106.29 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 14 | | 12 | | 15 | | HCH | | 107.37 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 107.28 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 10 | | 8 | | 11 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
| s 61 | 1.00 | | BEND | | 33 | | 28 | | 32 | | HCC | | 111.12 | | | f1333 13 | | | f1279 11 | | | f1259 13 | | |  | | |
| s 62 | 1.00 | | BEND | | 33 | | 28 | | 34 | | HCH | | 107.89 | | | f1481 73 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 30 | | 25 | | 31 | | HCH | | 105.73 | | |  | | |  | | |  | | |  | | |
| s 63 | 1.00 | | BEND | | 35 | | 29 | | 32 | | HCC | | 109.87 | | | f1374 11 | | | f1259 18 | | |  | | |  | | |
| s 64 | -1.00 | | BEND | | 26 | | 23 | | 27 | | HCH | | 107.42 | | | f1489 77 | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 11 | | HCH | | 107.28 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 35 | | 29 | | 36 | | HCH | | 106.01 | | |  | | |  | | |  | | |  | | |
| s 65 | 1.00 | | BEND | | 37 | | 32 | | 29 | | HCC | | 108.43 | | | f1379 11 | | | f1333 19 | | | f1279 12 | | | f1209 11 | | |
| s 66 | 1.00 | | BEND | | 37 | | 32 | | 38 | | HCH | | 105.93 | | | f1502 53 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 33 | | 28 | | 34 | | HCH | | 107.89 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 17 | | 16 | | 19 | | HCH | | 108.13 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 26 | | 23 | | 27 | | HCH | | 107.42 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 17 | | 16 | | 18 | | HCH | | 107.17 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 9 | | 8 | | 10 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
|  | -1.00 | |  | | 10 | | 8 | | 11 | | HCH | | 107.30 | | |  | | |  | | |  | | |  | | |
| s 67 | 1.00 | | BEND | | 28 | | 24 | | 41 | | CCO | | 120.91 | | | f606 18 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 28 | | 24 | | 42 | | CCN | | 117.22 | | |  | | |  | | |  | | |  | | |
| s 68 | 1.00 | | BEND | | 3 | | 4 | | 5 | | CCC | | 121.05 | | | f547 12 | | | f473 13 | | |  | | |  | | |
|  | 1.00 | |  | | 28 | | 24 | | 41 | | CCO | | 120.91 | | |  | | |  | | |  | | |  | | |
| s 69 | 1.00 | | BEND | | 6 | | 5 | | 4 | | CCC | | 121.18 | | | f919 13 | | | f473 11 | | |  | | |  | | |
| s 70 | 1.00 | | BEND | | 28 | | 24 | | 41 | | CCO | | 120.91 | | | f456 35 | | |  | | |  | | |  | | |
| s 71 | -1.00 | | BEND | | 4 | | 3 | | 16 | | CCC | | 119.68 | | | f346 70 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 5 | | 4 | | 39 | | CCO | | 120.96 | | |  | | |  | | |  | | |  | | |
| s 72 | 1.00 | | BEND | | 8 | | 6 | | 5 | | CCC | | 117.96 | | | f574 10 | | | f332 24 | | | f316 26 | | |  | | |
| s 73 | 1.00 | | BEND | | 12 | | 2 | | 3 | | CCC | | 118.37 | | | f574 11 | | | f388 29 | | | f368 10 | | |  | | |
| s 74 | 1.00 | | BEND | | 5 | | 4 | | 39 | | CCO | | 120.96 | | | f606 12 | | | f574 20 | | | f316 17 | | |  | | |
|  | 1.00 | |  | | 4 | | 3 | | 16 | | CCC | | 119.68 | | |  | | |  | | |  | | |  | | |
| s 75 | 1.00 | | BEND | | 20 | | 1 | | 2 | | CCC | | 119.99 | | |  | | |  | | |  | | |  | | |
| s 76 | 1.00 | | BEND | | 42 | | 20 | | 1 | | NCC | | 112.05 | | | f49 23 | | |  | | |  | | |  | | |
| s 77 | 1.00 | | BEND | | 20 | | 42 | | 24 | | CNC | | 120.58 | | | f204 39 | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 28 | | 24 | | 42 | | CCN | | 117.22 | | |  | | |  | | |  | | |  | | |
| s 78 | 1.00 | | BEND | | 20 | | 42 | | 24 | | CNC | | 120.58 | | |  | | |  | | |  | | |  | | |
|  | 1.00 | |  | | 23 | | 42 | | 24 | | CNC | | 110.94 | | |  | | |  | | |  | | |  | | |
| s 79 | 1.00 | | BEND | | 25 | | 23 | | 42 | | CCN | | 112.22 | | | f858 11 | | | f515 20 | | |  | | |  | | |
| s 80 | 1.00 | | BEND | | 29 | | 25 | | 23 | | CCC | | 116.24 | | | f869 11 | | |  | | |  | | |  | | |
| s 81 | 1.00 | | BEND | | 32 | | 29 | | 25 | | CCC | | 116.18 | | | f1014 11 | | | f515 10 | | | f423 15 | | |  | | |
| s 82 | 1.00 | TORS | | 40 | | 39 | | 4 | | 5 | | HOCC | | | -1.49 | | | f307 51 | | | f291 17 | | | f286 15 | | |
| s 83 | 1.00 | TORS | | 7 | | 5 | | 4 | | 3 | | HCCC | | | -180.73 | | | f840 61 | | |  | | |  | | |
| s 84 | -1.00 | TORS | | 10 | | 8 | | 6 | | 5 | | HCCC | | | -118.08 | | | f1058 36 | | |  | | |  | | |
|  | 1.00 |  | | 9 | | 8 | | 6 | | 5 | | HCCC | | | 1.42 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -125.13 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -9.08 | | |  | | |  | | |  | | |
| s 85 | 1.00 | TORS | | 9 | | 8 | | 6 | | 5 | | HCCC | | | 1.42 | | | f1056 48 | | | f1027 10 | | |  | | |
|  | -1.00 |  | | 11 | | 8 | | 6 | | 5 | | HCCC | | | -238.96 | | |  | | |  | | |  | | |
| s 86 | 1.00 | TORS | | 11 | | 8 | | 6 | | 5 | | HCCC | | | -238.96 | | | f209 11 | | | f160 55 | | | f155 19 | | |
| s 87 | 1.00 | TORS | | 18 | | 16 | | 3 | | 2 | | HCCC | | | -70.17 | | | f155 16 | | | f136 30 | | | f121 11 | | |
|  | 1.00 |  | | 19 | | 16 | | 3 | | 2 | | HCCC | | | -189.96 | | |  | | |  | | |  | | |
| s 88 | 1.00 | TORS | | 14 | | 12 | | 2 | | 1 | | HCCC | | | -30.99 | | | f1037 48 | | |  | | |  | | |
|  | -1.00 |  | | 19 | | 16 | | 3 | | 2 | | HCCC | | | -189.96 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -151.25 | | |  | | |  | | |  | | |
| s 89 | 1.00 | TORS | | 13 | | 12 | | 2 | | 1 | | HCCC | | | 88.25 | | | f105 12 | | | f98 71 | | |  | | |
|  | 1.00 |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -151.25 | | |  | | |  | | |  | | |
| s 90 | -1.00 | TORS | | 17 | | 16 | | 3 | | 2 | | HCCC | | | 49.61 | | | f1069 50 | | |  | | |  | | |
|  | 1.00 |  | | 14 | | 12 | | 2 | | 1 | | HCCC | | | -30.99 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -151.25 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 19 | | 16 | | 3 | | 2 | | HCCC | | | -189.96 | | |  | | |  | | |  | | |
| s 91 | 1.00 | TORS | | 10 | | 8 | | 6 | | 5 | | HCCC | | | -118.08 | | | f1027 32 | | |  | | |  | | |
|  | -1.00 |  | | 14 | | 12 | | 2 | | 1 | | HCCC | | | -30.99 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 9 | | 8 | | 6 | | 5 | | HCCC | | | 1.42 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 13 | | 12 | | 2 | | 1 | | HCCC | | | 88.25 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 18 | | 16 | | 3 | | 2 | | HCCC | | | -70.17 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -9.08 | | |  | | |  | | |  | | |
| s 92 | 1.00 | TORS | | 13 | | 12 | | 2 | | 1 | | HCCC | | | 88.25 | | | f1098 35 | | |  | | |  | | |
|  | -1.00 |  | | 18 | | 16 | | 3 | | 2 | | HCCC | | | -70.17 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 15 | | 12 | | 2 | | 1 | | HCCC | | | -151.25 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 17 | | 16 | | 3 | | 2 | | HCCC | | | 49.61 | | |  | | |  | | |  | | |
| s 93 | -1.00 | TORS | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -125.13 | | | f1395 15 | | | f1391 30 | | |  | | |
|  | 1.00 |  | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -9.08 | | |  | | |  | | |  | | |
| s 94 | 1.00 | TORS | | 9 | | 8 | | 6 | | 5 | | HCCC | | | 1.42 | | | f1000 11 | | | f974 13 | | |  | | |
|  | -1.00 |  | | 10 | | 8 | | 6 | | 5 | | HCCC | | | -118.08 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 13 | | 12 | | 2 | | 1 | | HCCC | | | 88.25 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 14 | | 12 | | 2 | | 1 | | HCCC | | | -30.99 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 21 | | 20 | | 1 | | 6 | | HCCC | | | -9.08 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -125.13 | | |  | | |  | | |  | | |
| s 95 | -1.00 | TORS | | 22 | | 20 | | 1 | | 6 | | HCCC | | | -125.13 | | | f1382 51 | | |  | | |  | | |
|  | 1.00 |  | | 26 | | 23 | | 42 | | 20 | | HCNC | | | -195.72 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 27 | | 23 | | 42 | | 20 | | HCNC | | | 48.38 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 35 | | 29 | | 32 | | 28 | | HCCC | | | 45.98 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 36 | | 29 | | 32 | | 28 | | HCCC | | | -199.29 | | |  | | |  | | |  | | |
| s 96 | 1.00 | TORS | | 26 | | 23 | | 42 | | 20 | | HCNC | | | -195.72 | | | f1395 11 | | | f1379 10 | | |  | | |
|  | 1.00 |  | | 35 | | 29 | | 32 | | 28 | | HCCC | | | 45.98 | | |  | | |  | | |  | | |
| s 97 | 1.00 | TORS | | 30 | | 25 | | 29 | | 32 | | HCCC | | | -54.49 | | | f815 13 | | |  | | |  | | |
|  | -1.00 |  | | 36 | | 29 | | 32 | | 28 | | HCCC | | | -199.29 | | |  | | |  | | |  | | |
| s 98 | 1.00 | TORS | | 34 | | 28 | | 24 | | 42 | | HCCN | | | -61.28 | | | f1209 37 | | |  | | |  | | |
| s 99 | 1.00 | TORS | | 33 | | 28 | | 24 | | 42 | | HCCN | | | -180.12 | | | f717 10 | | |  | | |  | | |
| s 100 | 1.00 | TORS | | 31 | | 25 | | 29 | | 32 | | HCCC | | | -168.83 | | | f1279 17 | | | f1209 11 | | |  | | |
|  | -1.00 |  | | 34 | | 28 | | 24 | | 42 | | HCCN | | | -61.28 | | |  | | |  | | |  | | |
| s 101 | -1.00 | TORS | | 27 | | 23 | | 42 | | 20 | | HCNC | | | 48.38 | | | f515 29 | | |  | | |  | | |
|  | 1.00 |  | | 35 | | 29 | | 32 | | 28 | | HCCC | | | 45.98 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 36 | | 29 | | 32 | | 28 | | HCCC | | | -199.29 | | |  | | |  | | |  | | |
| s 102 | 1.00 | TORS | | 27 | | 23 | | 42 | | 20 | | HCNC | | | 48.38 | | | f1391 14 | | | f1374 14 | | |  | | |
|  | 1.00 |  | | 36 | | 29 | | 32 | | 28 | | HCCC | | | -199.29 | | |  | | |  | | |  | | |
| s 103 | 1.00 | TORS | | 37 | | 32 | | 29 | | 25 | | HCCC | | | -200.89 | | | f1014 10 | | |  | | |  | | |
| s 104 | 1.00 | TORS | | 38 | | 32 | | 29 | | 25 | | HCCC | | | 44.50 | | | f1374 13 | | | f1333 15 | | |  | | |
| s 105 | 1.00 | OUT | | 8 | | 1 | | 5 | | 6 | | CCCC | | | 0.56 | | | f110 60 | | |  | | |  | | |
|  | 1.00 |  | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.15 | | |  | | |  | | |  | | |
|  | -1.00 | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.36 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.16 | | |  | | |  | | |  | | |
|  | -1.00 | OUT | | 39 | | 3 | | 5 | | 4 | | OCCC | | | 0.33 | | |  | | |  | | |  | | |
| s 106 | 1.00 | OUT | | 8 | | 1 | | 5 | | 6 | | CCCC | | | 0.56 | | | f549 57 | | |  | | |  | | |
|  | 1.00 |  | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.15 | | |  | | |  | | |  | | |
|  | 1.00 | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.36 | | |  | | |  | | |  | | |
|  | -1.00 | OUT | | 39 | | 3 | | 5 | | 4 | | OCCC | | | 0.33 | | |  | | |  | | |  | | |
| s 107 | -1.00 | OUT | | 8 | | 1 | | 5 | | 6 | | CCCC | | | 0.56 | | | f209 56 | | | f176 12 | | |  | | |
|  | 1.00 |  | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.15 | | |  | | |  | | |  | | |
|  | 1.00 | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.36 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.16 | | |  | | |  | | |  | | |
|  | 1.00 | OUT | | 39 | | 3 | | 5 | | 4 | | OCCC | | | 0.33 | | |  | | |  | | |  | | |
| s 108 | 1.00 | TORS | | 1 | | 20 | | 42 | | 24 | | CCNC | | | -212.82 | | | f58 71 | | |  | | |  | | |
|  | -1.00 |  | | 6 | | 1 | | 20 | | 42 | | CCCN | | | -243.87 | | |  | | |  | | |  | | |
| s 109 | 1.00 | TORS | | 28 | | 24 | | 42 | | 20 | | CCNC | | | 34.99 | | | f858 10 | | | f136 11 | | | f121 17 | | |
| s 110 | 1.00 | TORS | | 1 | | 20 | | 42 | | 24 | | CCNC | | | -212.82 | | | f19 80 | | |  | | |  | | |
|  | 1.00 |  | | 6 | | 1 | | 20 | | 42 | | CCCN | | | -243.87 | | |  | | |  | | |  | | |
| s 111 | 1.00 | TORS | | 20 | | 42 | | 23 | | 25 | | CNCC | | | -74.29 | | | f176 22 | | |  | | |  | | |
|  | -1.00 |  | | 29 | | 25 | | 23 | | 42 | | CCCN | | | -48.75 | | |  | | |  | | |  | | |
| s 112 | 1.00 | TORS | | 20 | | 42 | | 23 | | 25 | | CNCC | | | -74.29 | | | f105 43 | | |  | | |  | | |
|  | 1.00 |  | | 29 | | 25 | | 23 | | 42 | | CCCN | | | -48.75 | | |  | | |  | | |  | | |
| s 113 | 1.00 | TORS | | 32 | | 29 | | 25 | | 23 | | CCCC | | | 69.66 | | | f1129 10 | | | f1000 11 | | |  | | |
| s 114 | 1.00 | OUT | | 41 | | 28 | | 42 | | 24 | | OCNC | | | 10.55 | | | f717 10 | | | f121 14 | | |  | | |
| s 115 | 1.00 | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.36 | | | f840 19 | | | f757 11 | | | f286 10 | | |
|  | 1.00 |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.16 | | |  | | |  | | |  | | |
|  | -1.00 |  | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.90 | | |  | | |  | | |  | | |
| s 116 | 1.00 | OUT | | 16 | | 2 | | 4 | | 3 | | CCCC | | | 0.17 | | | f396 10 | | | f286 18 | | |  | | |
| s 117 | 1.00 | OUT | | 12 | | 1 | | 3 | | 2 | | CCCC | | | 0.15 | | | f651 28 | | | f606 11 | | | f396 17 | | |
|  | -1.00 |  | | 39 | | 3 | | 5 | | 4 | | OCCC | | | 0.33 | | |  | | |  | | |  | | |
| s 118 | 1.00 | OUT | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.24 | | | f49 52 | | |  | | |  | | |
|  | 1.00 | TORS | | 1 | | 6 | | 5 | | 4 | | CCCC | | | 0.36 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 2 | | 3 | | 4 | | 5 | | CCCC | | | -0.16 | | |  | | |  | | |  | | |
|  | 1.00 |  | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.90 | | |  | | |  | | |  | | |
| s 119 | 1.00 | OUT | | 23 | | 20 | | 24 | | 42 | | CCCN | | | 35.46 | | |  | | |  | | |  | | |
| s 120 | -1.00 | OUT | | 20 | | 2 | | 6 | | 1 | | CCCC | | | 0.24 | | | f396 13 | | | f155 16 | | | f121 10 | | |
|  | 1.00 | TORS | | 3 | | 4 | | 5 | | 6 | | CCCC | | | -0.90 | | |  | | |  | | |  | | |