

# **ESI of**

## **Gas phase acidity of water clusters**

Amit Kumar and Pradeep Kumar\*

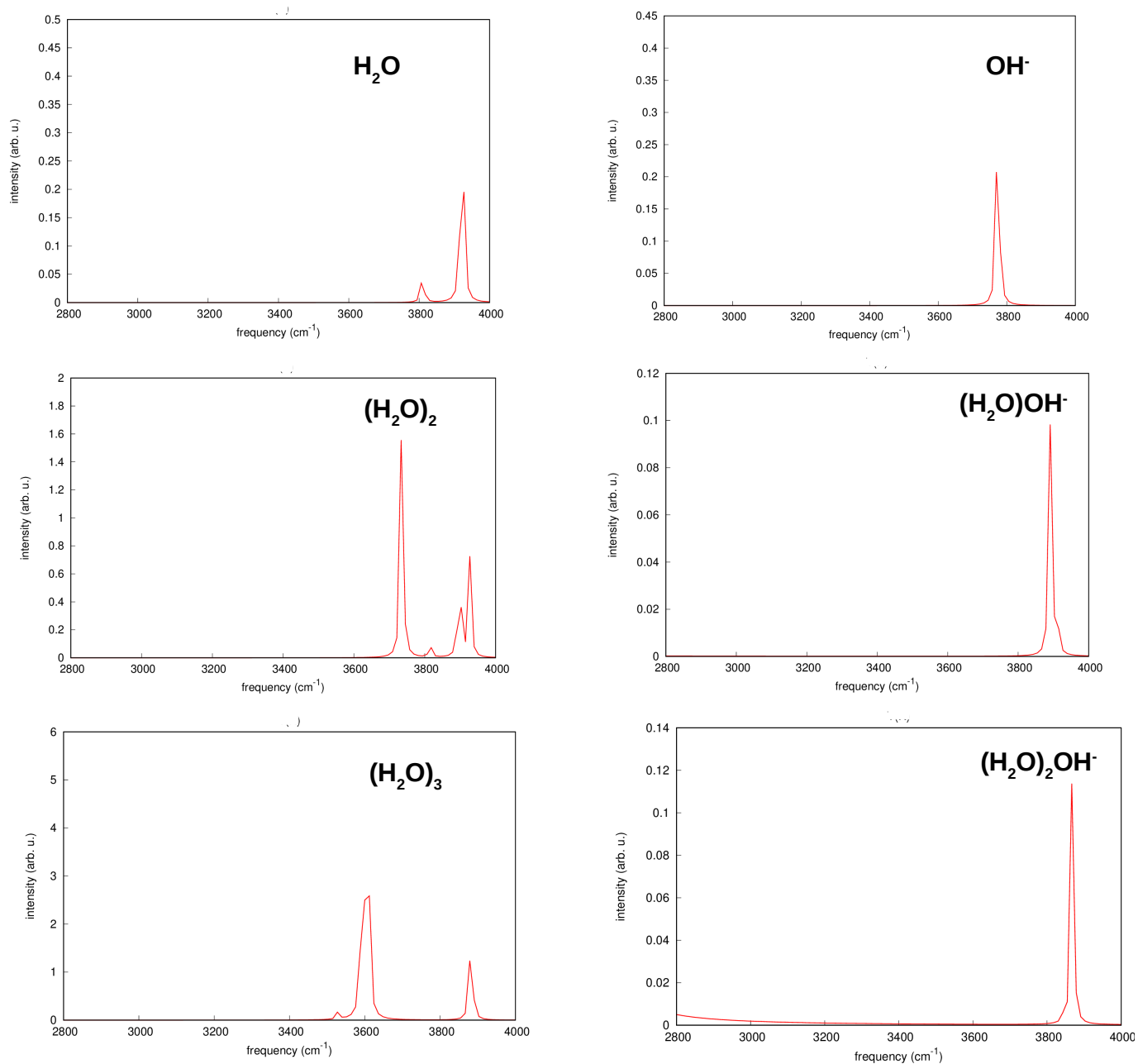
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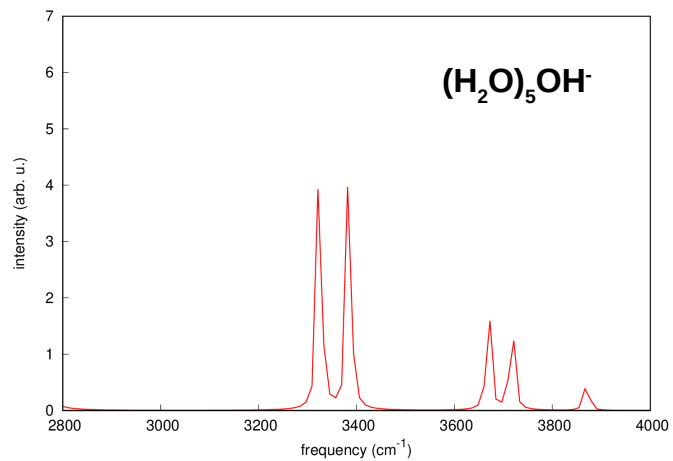
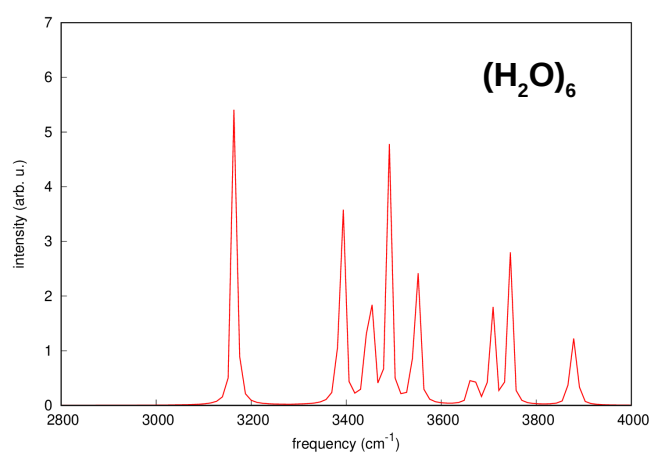
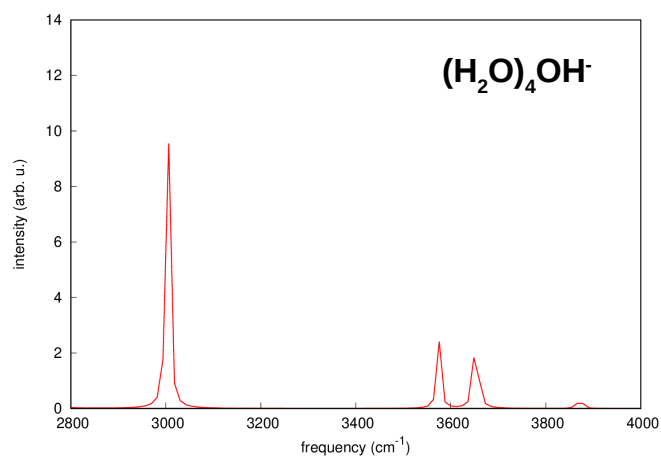
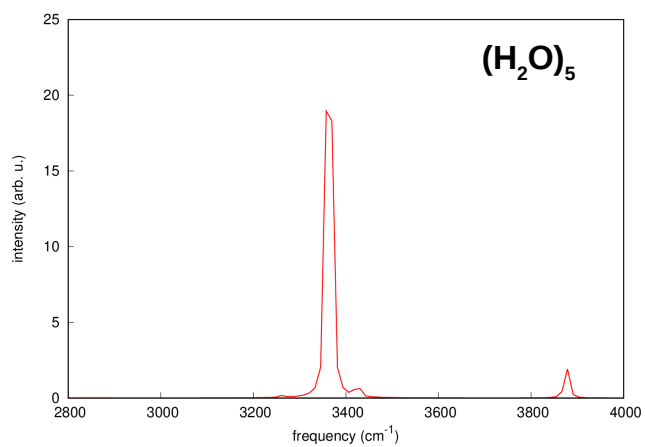
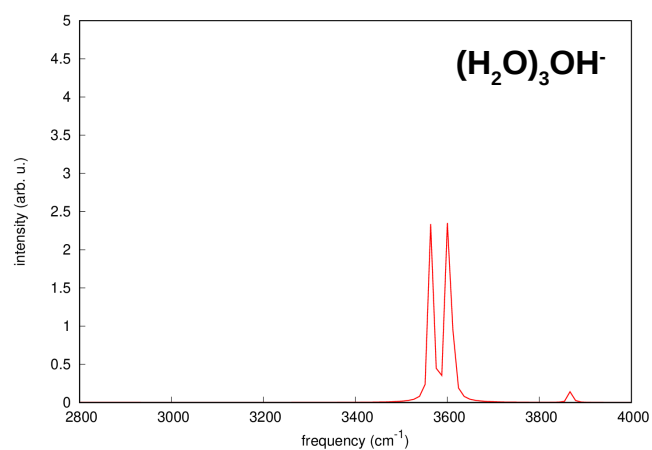
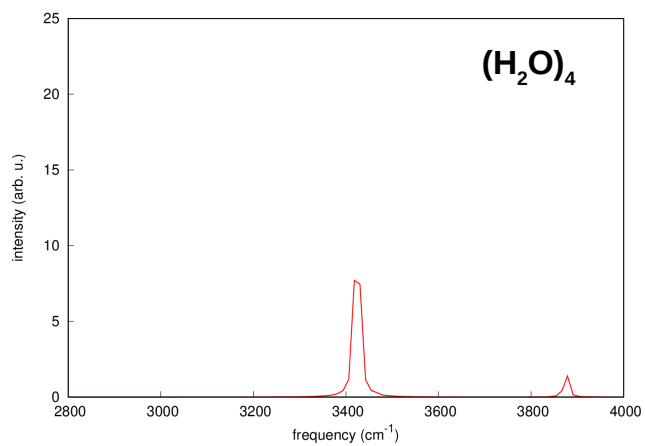
E-mail: [pradeep.chy@mnit.ac.in](mailto:pradeep.chy@mnit.ac.in)

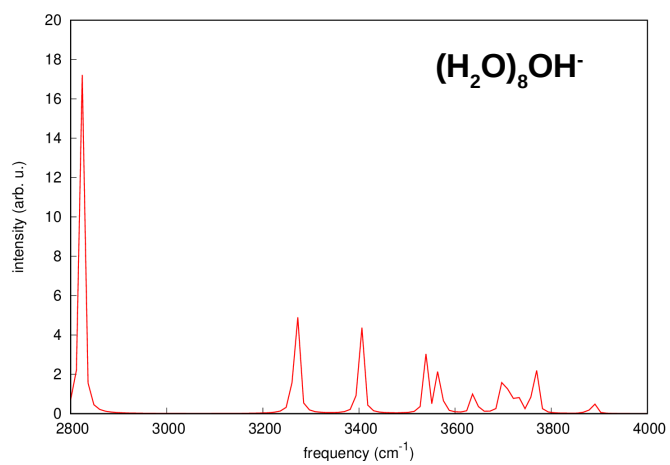
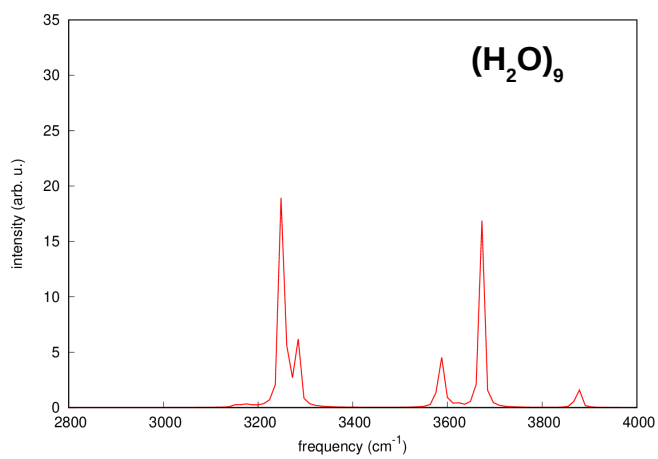
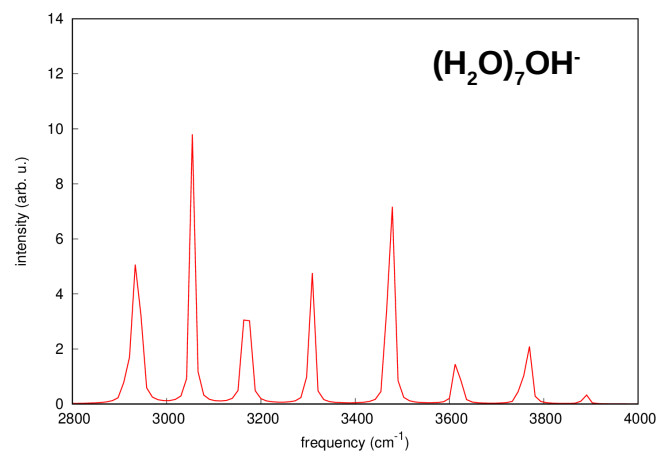
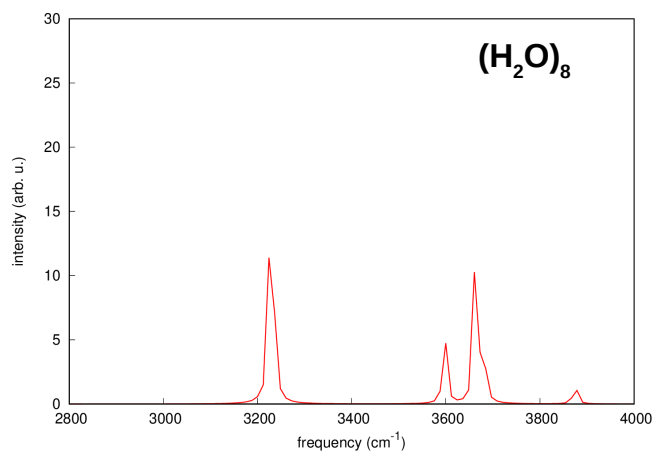
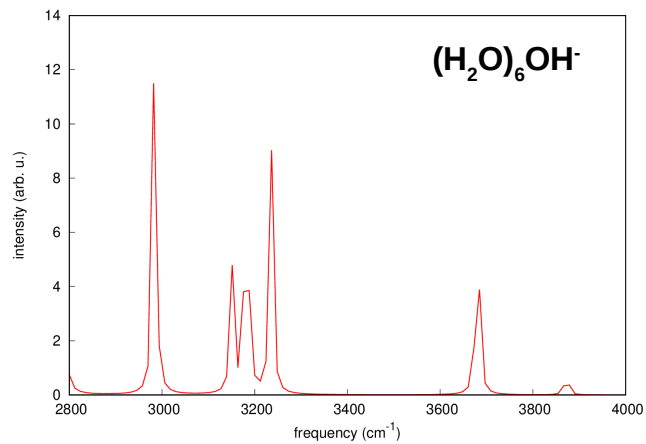
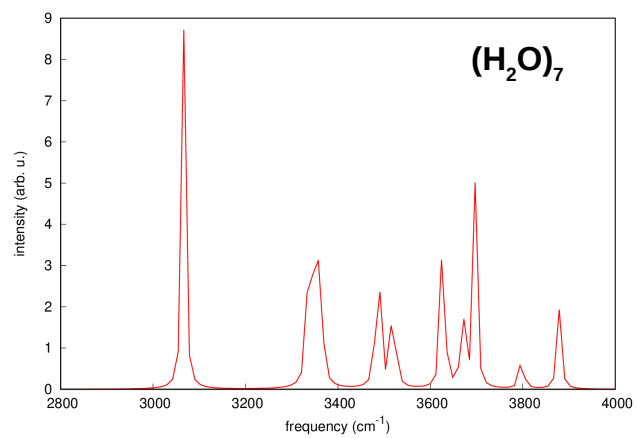
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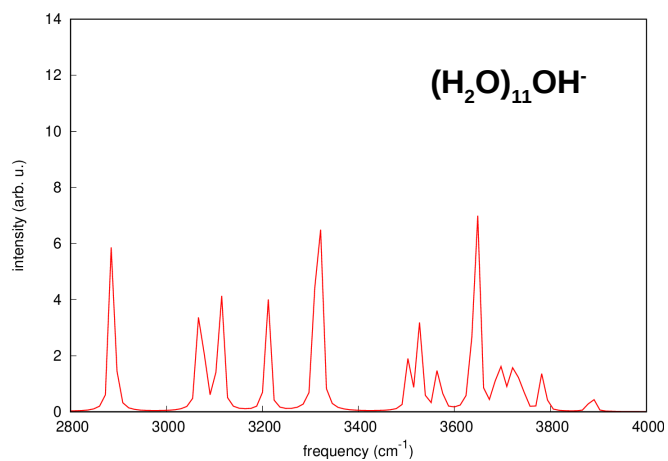
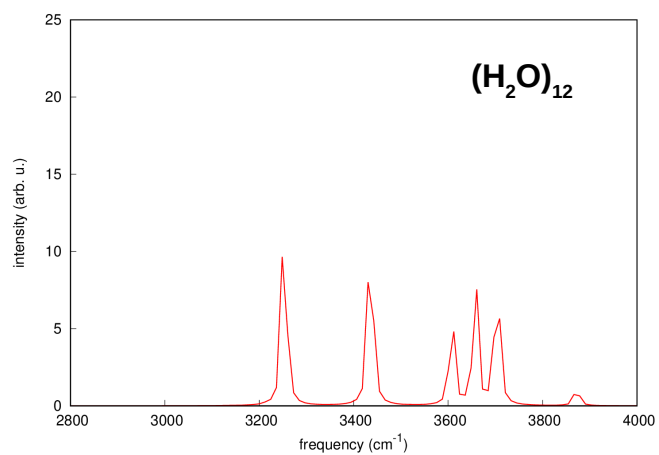
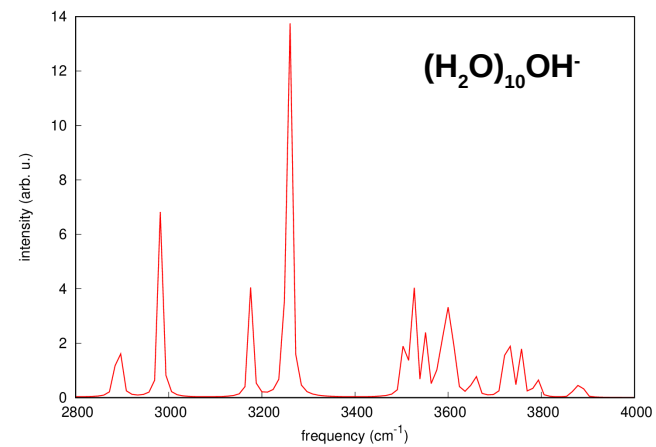
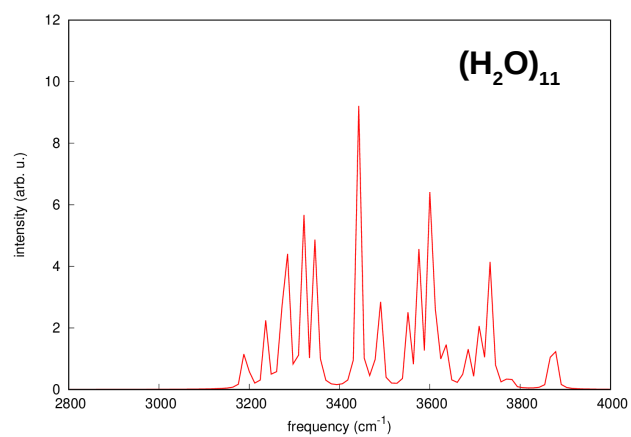
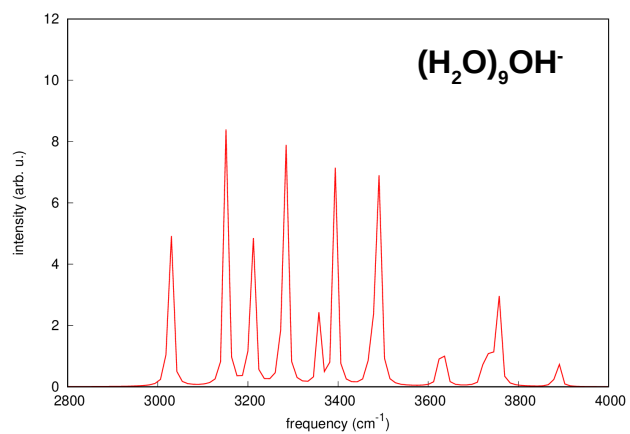
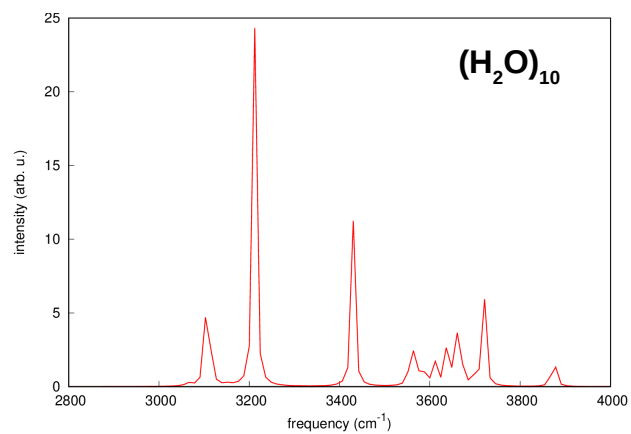
1. **Figure S1:** IR spectra of different water cluster and there corresponding deprotonated water cluster estimated at B3LYP/6-31+G(2d,p) level of theory.
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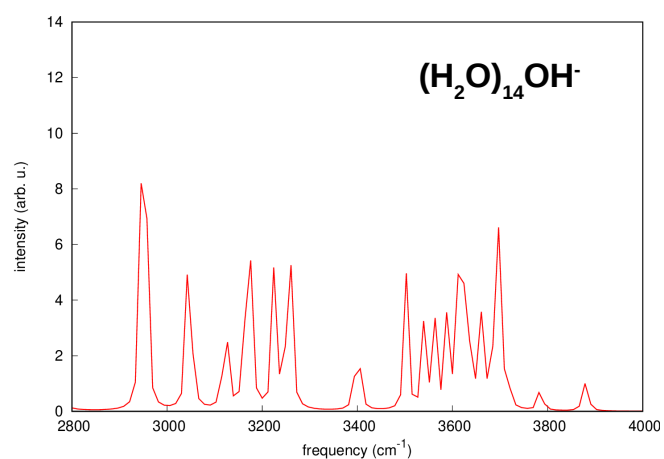
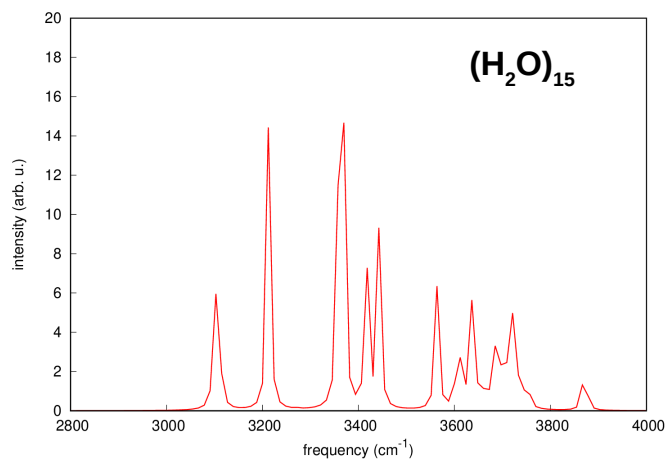
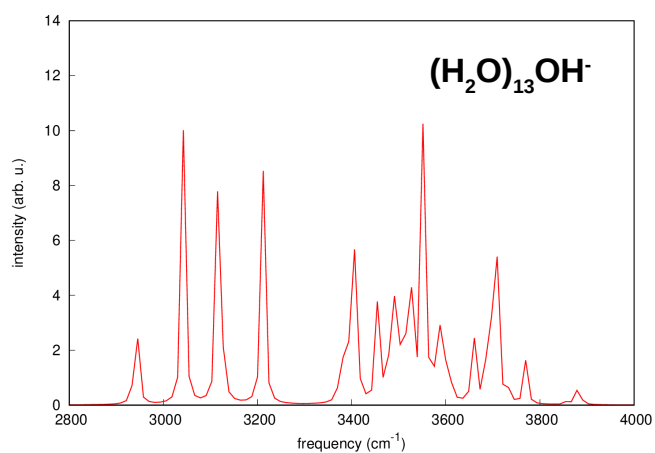
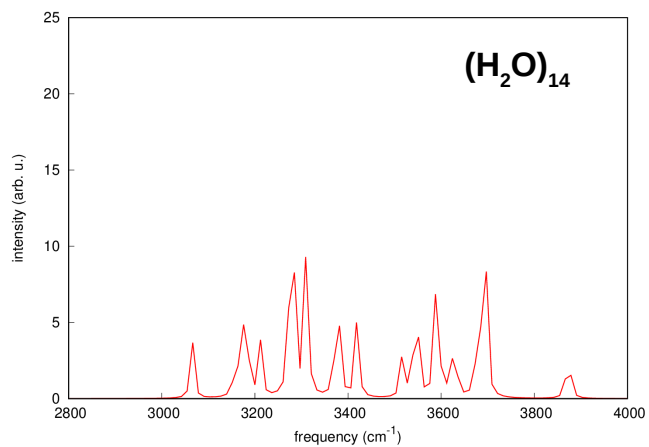
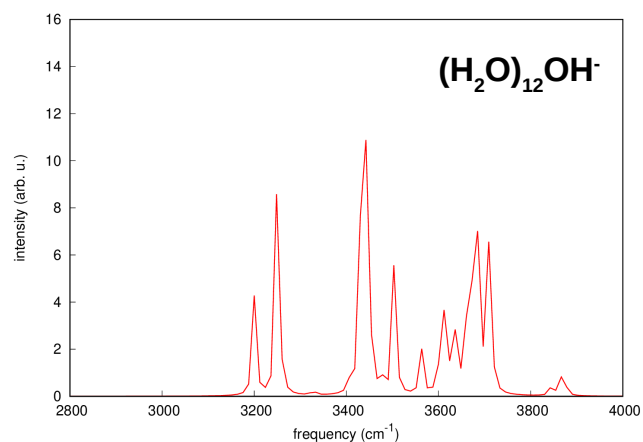
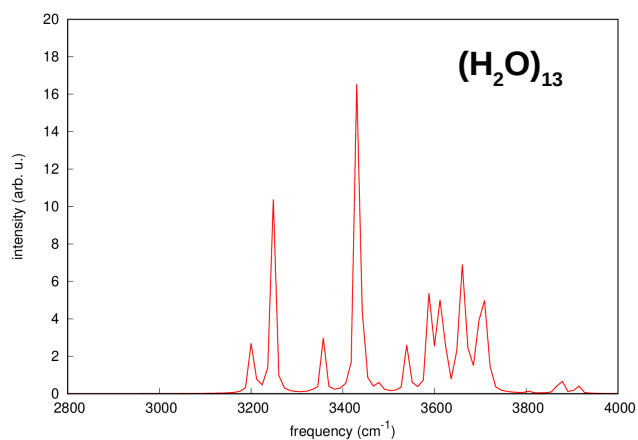
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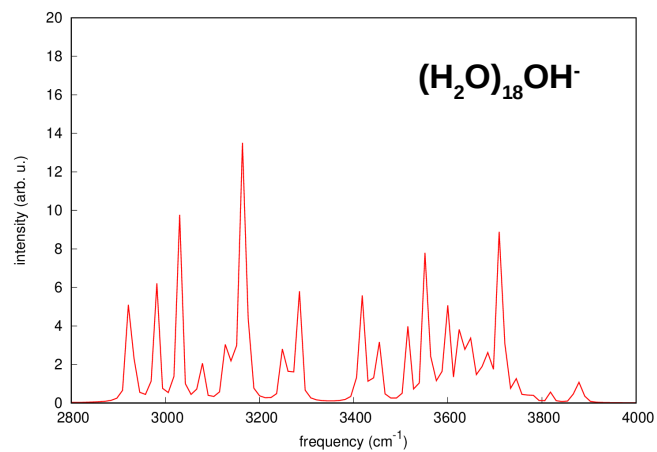
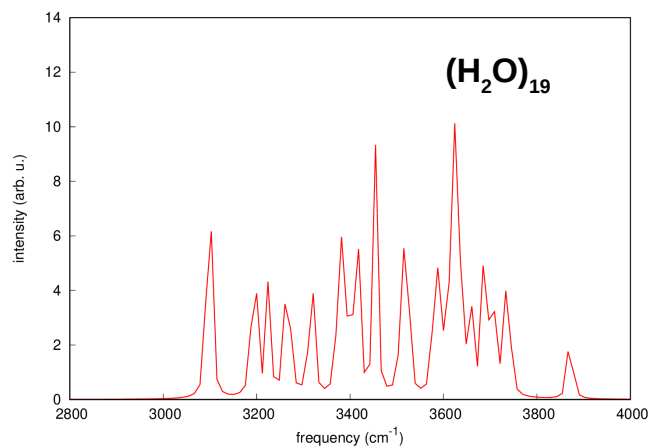
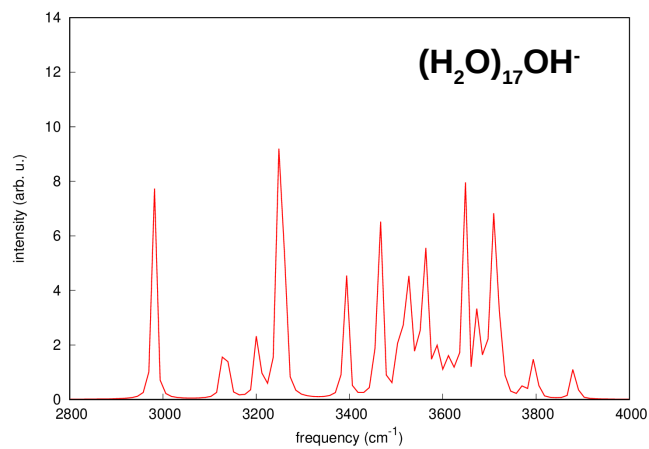
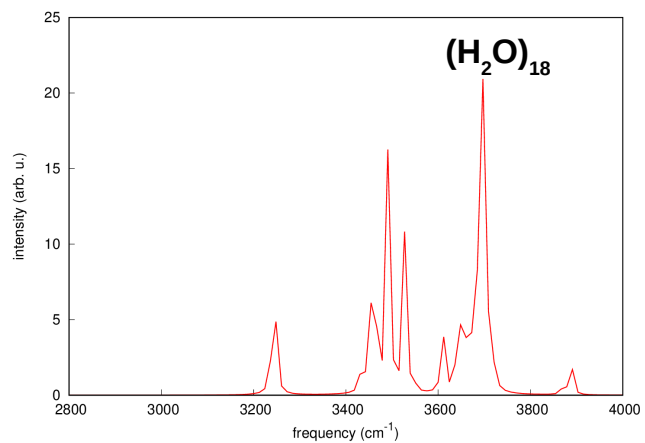
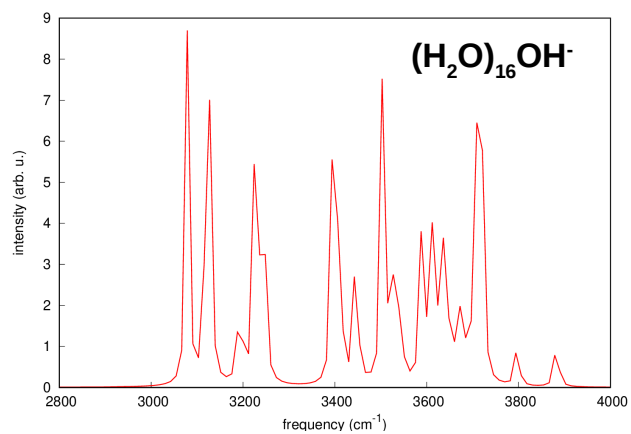
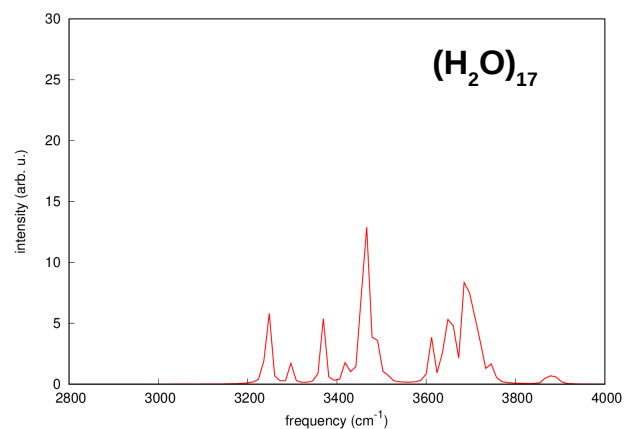


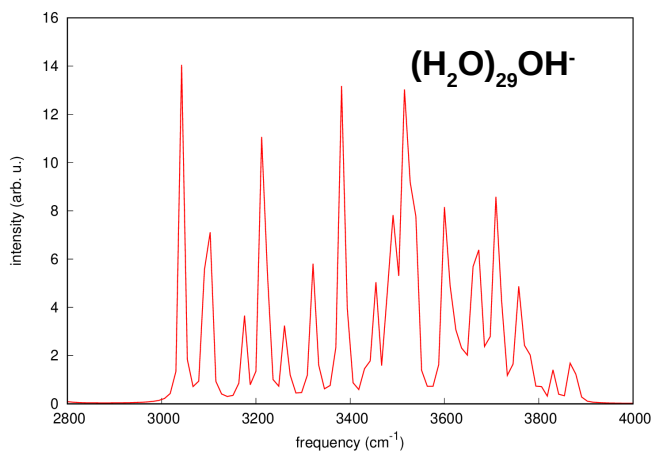
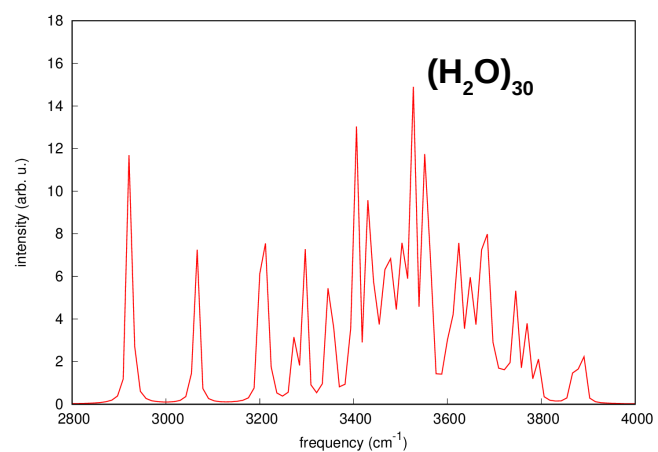
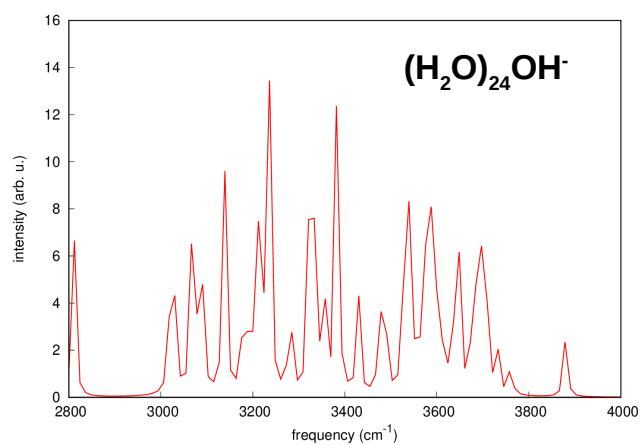
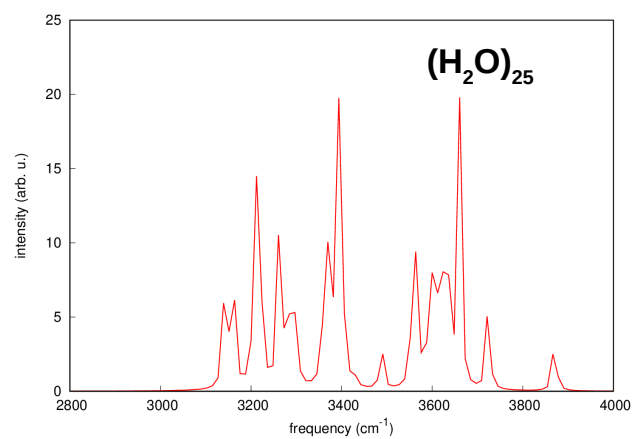
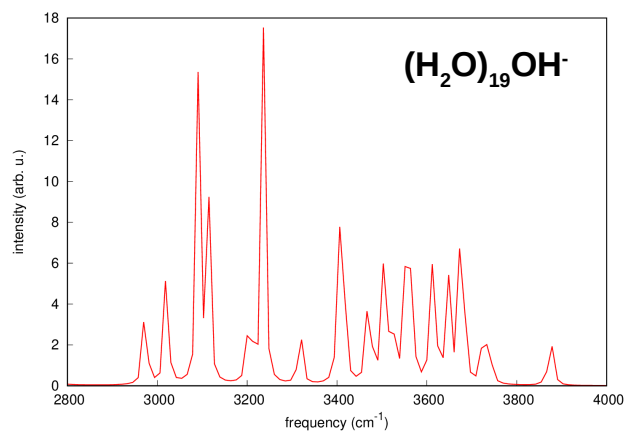
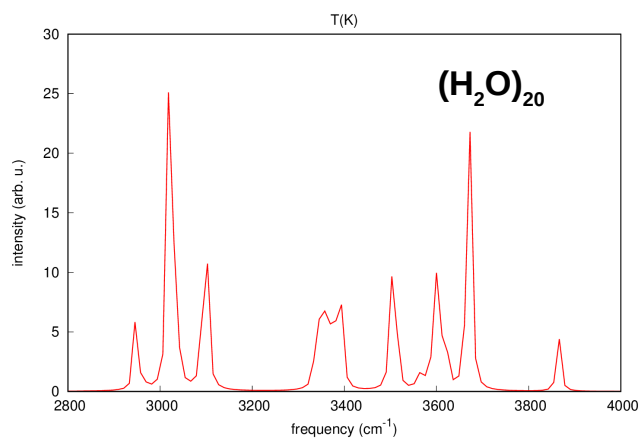


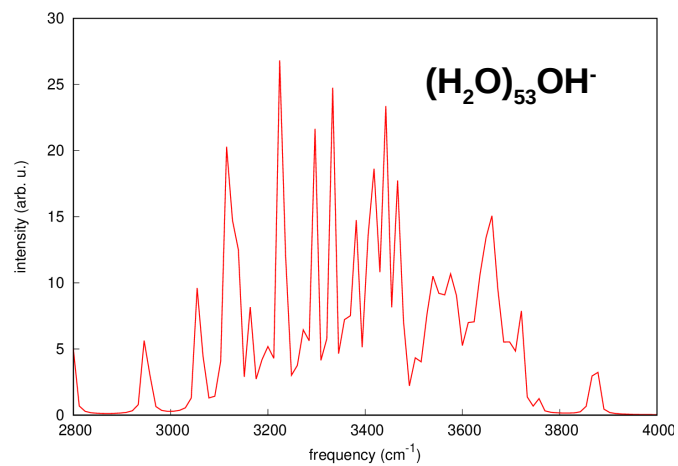
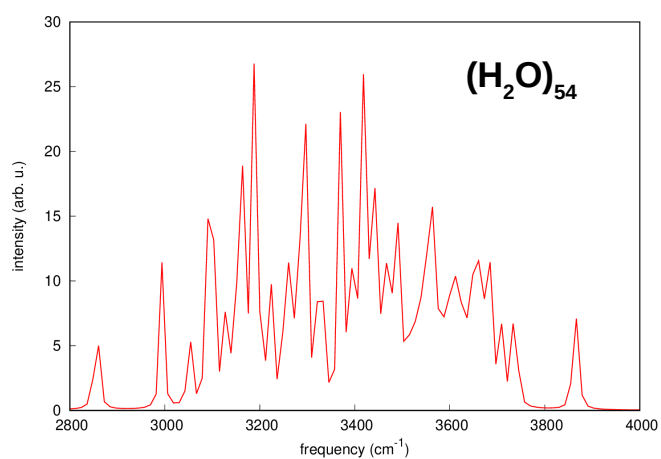
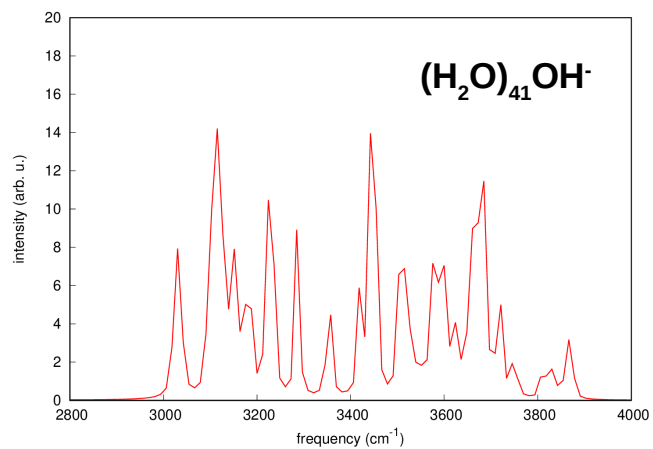
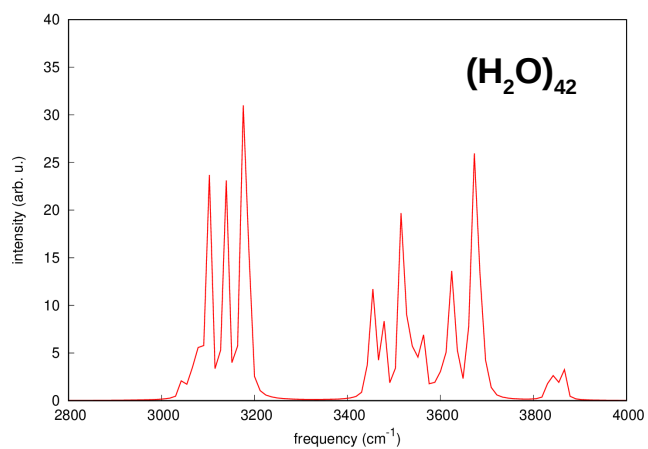
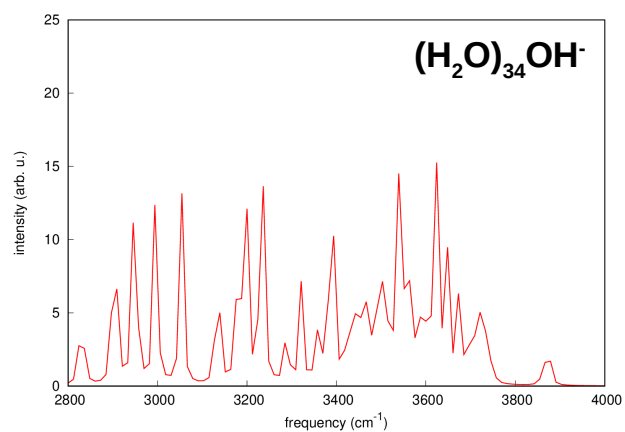
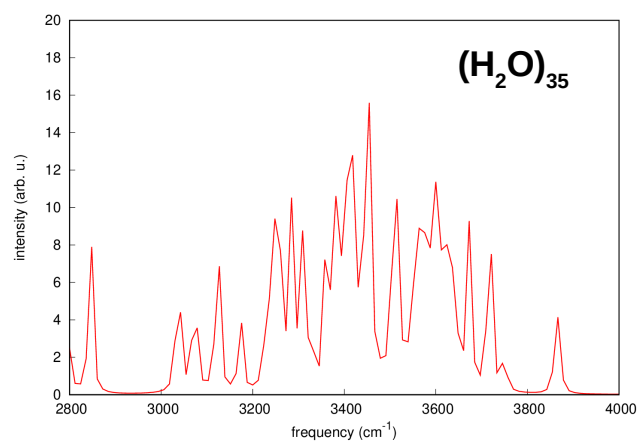












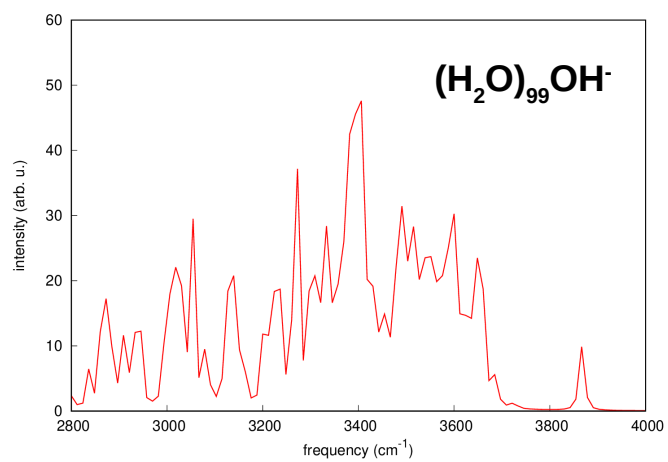
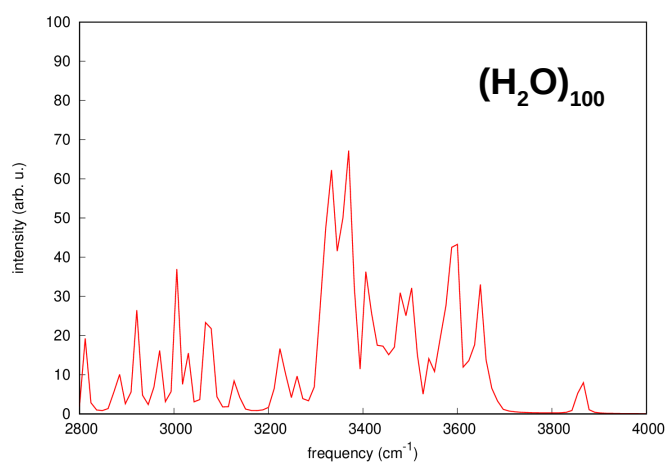
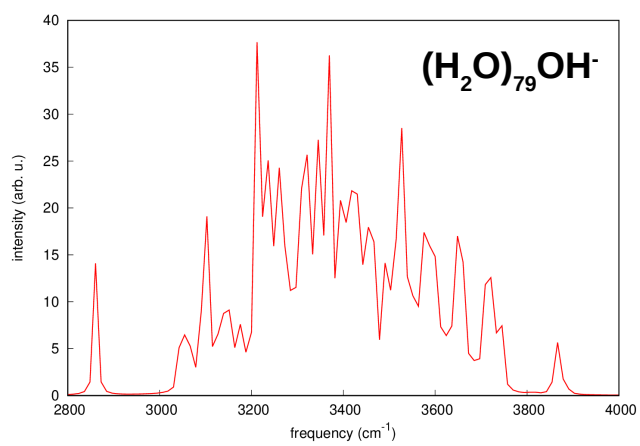
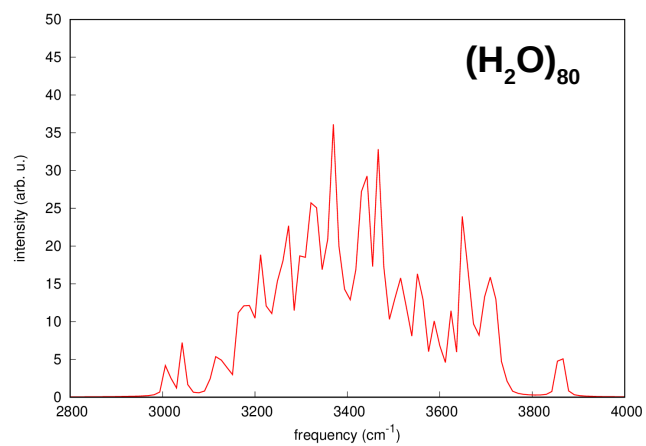


Table S1: Binding energies of water clusters (n=2-6) in kcal mol<sup>-1</sup> at different DFT functionals

| n | MP2/CBS      | M06-2X/6-31++G(d,p) | X3-LYP/6-31+G(2d,p) | M052X/6-31+G(2d,p) | M06-L/6-31+G(2d,p) | B3LYP/6-311++G(2d,2p) | BLYP/6-31+G(2d,p) |
|---|--------------|---------------------|---------------------|--------------------|--------------------|-----------------------|-------------------|
| 2 | <b>-4.8</b>  | -5.98               | -4.60               | -4.77              | -4.08              | -4.19                 | -4.22             |
| 3 | <b>-15.3</b> | -20.63              | -16.71              | -17.43             | -16.21             | -15.33                | -15.59            |
| 4 | <b>-27.1</b> | -34.62              | -29.81              | -29.53             | -27.78             | -27.42                | -28.07            |
| 5 | <b>-35.6</b> | -45.06              | -39.15              | -38.27             | -35.75             | -36.14                | -36.89            |
| 6 | <b>-45.1</b> | -59.13              | -48.00              | -49.95             | -47.13             | -44.08                | -44.81            |

Table S2: Comparison of geometrical parameters of H<sub>2</sub>O and (H<sub>2</sub>O)<sub>2</sub> between Experimental and higher level calculation with B3LYP/6-31+G(2d,p) level of theory alongwith harmonic frequencies.

| Species                         | Parameters                      | Expt. <sup>1</sup> | CCSD(T)/aug-cc-pVTZ | B3LYP/6-31+G(2d,p) |
|---------------------------------|---------------------------------|--------------------|---------------------|--------------------|
| H <sub>2</sub> O                | O-H (Å)                         | 0.95               | 0.96                | 0.96               |
|                                 | O-H-O (deg.)                    | 104.52             | 104.18              | 105.28             |
|                                 | frequencies (cm <sup>-1</sup> ) | 1648               | 1646                | 1635               |
|                                 |                                 | 3832               | 3810                | 3810               |
|                                 |                                 | 3943               | 3919                | 3922               |
| (H <sub>2</sub> O) <sub>2</sub> | O-O (Å)                         | 2.97               | 2.91                | 2.95               |
|                                 | frequencies (cm <sup>-1</sup> ) | 3718               | 3730                | 3735               |
|                                 |                                 | 3797               | 3805                | 3815               |
|                                 |                                 | 3881               | 3889                | 3898               |
|                                 |                                 | 3899               | 3911                | 3927               |

Table S3: Comparison of frequencies ( in  $\text{cm}^{-1}$ ) obtained from harmonic and anharmonic calculation at B3LYP/6-31+G(2d,p) level of theory with experimental values.

| n                        | harm | anharm | Exp. <sup>1-3</sup> |
|--------------------------|------|--------|---------------------|
| $\text{H}_2\text{O}$     | 3810 | 3640   | 3657                |
|                          | 1635 | 1582   | 1595                |
|                          | 3922 | 3737   | 3756                |
| $(\text{H}_2\text{O})_2$ | 3928 | 3689   | 3745                |
|                          | 3897 | 3666   | 3735                |
|                          | 3815 | 3611   | 3660                |
|                          | 3733 | 3562   | 3601                |
| $(\text{H}_2\text{O})_3$ | 3885 | 3717   | 3726                |
|                          | 3884 | 3692   | 3726                |
|                          | 3608 | 3477   | 3530                |
|                          | 3595 | 3447   | 3532                |
|                          | 3529 | 3376   | 3472                |
|                          | 1674 | 1623   | 1638                |
|                          | 1652 | 1603   | 1609                |
|                          | 696  | 596    | 578                 |
|                          | 603  | 472    | 458                 |
|                          | 464  | 399    | 434                 |
|                          | 380  | 216    | 414                 |
|                          | 359  | 353    | 386                 |
|                          | 266  | 429    | 353                 |
|                          | 183  | 164    | 170                 |
| $(\text{H}_2\text{O})_4$ | 3877 | 3701   | 3714                |
|                          | 3466 | 3321   | 3416                |
| $(\text{H}_2\text{O})_5$ | 3880 | 3704   | 3714                |
|                          | 3428 | 3333   | 3360                |

Table S4: Comparison of gas phase acidity estimated from harmonic and anharmonic calculation for different water cluster.

| n | $\Delta H$ (kj mol <sup>-1</sup> ) |         |
|---|------------------------------------|---------|
|   | harm                               | anharm  |
| 2 | 1522.19                            | 1510.64 |
| 3 | 1473.37                            | 1474.52 |
| 4 | 1455.96                            | 1457.17 |
| 5 | 1440.47                            | 1439.76 |
| 6 | 1390.59                            | 1395.21 |

Table S5: Absolute value of G, H, and S for  $(\text{H}_2\text{O})_n$  and  $(\text{H}_2\text{O})_{n-1}\text{OH}^-$  species for different water cluster.

| n   | H ( $\text{kJ mol}^{-1}$ ) |                                         | G ( $\text{kJ mol}^{-1}$ ) |                                         | S ( $\text{J mol}^{-1} \text{K}^{-1}$ ) |                                         |
|-----|----------------------------|-----------------------------------------|----------------------------|-----------------------------------------|-----------------------------------------|-----------------------------------------|
|     | $(\text{H}_2\text{O})_n$   | $(\text{H}_2\text{O})_{n-1}\text{OH}^-$ | $(\text{H}_2\text{O})_n$   | $(\text{H}_2\text{O})_{n-1}\text{OH}^-$ | $(\text{H}_2\text{O})_n$                | $(\text{H}_2\text{O})_{n-1}\text{OH}^-$ |
| 1   | -200435.97                 | -198812.69                              | -200492.17                 | -198863.99                              | 188.58                                  | 172.18                                  |
| 2   | -400888.22                 | -399373.66                              | -400969.41                 | -399447.32                              | 272.43                                  | 247.19                                  |
| 3   | -601357.43                 | -599891.60                              | -601456.03                 | -599991.47                              | 330.88                                  | 335.13                                  |
| 4   | -801837.70                 | -800393.96                              | -801951.24                 | -800504.18                              | 381.00                                  | 369.86                                  |
| 5   | -1002303.98                | -1000878.05                             | -1002439.44                | -1001011.08                             | 454.57                                  | 446.41                                  |
| 6   | -1202763.93                | -1201345.30                             | -1202908.83                | -1201490.11                             | 486.25                                  | 485.93                                  |
| 7   | -1403239.51                | -1401852.96                             | -1403398.20                | -1402009.26                             | 532.50                                  | 524.49                                  |
| 8   | -1603729.02                | -1602340.13                             | -1603893.76                | -1602503.15                             | 552.80                                  | 547.06                                  |
| 9   | -1804197.99                | -1802798.21                             | -1804380.37                | -1802981.98                             | 612.03                                  | 616.66                                  |
| 10  | -2004672.14                | -2003288.78                             | -2004866.33                | -2003483.12                             | 651.65                                  | 652.14                                  |
| 11  | -2205119.21                | -2203753.83                             | -2205336.14                | -2203965.82                             | 727.96                                  | 711.38                                  |
| 12  | -2405613.81                | -2404239.73                             | -2405832.30                | -2404458.97                             | 733.19                                  | 735.73                                  |
| 13  | -2606065.38                | -2604708.67                             | -2606313.58                | -2604951.75                             | 832.88                                  | 815.70                                  |
| 14  | -2806544.79                | -2805226.83                             | -2806806.44                | -2805468.97                             | 878.00                                  | 812.56                                  |
| 15  | -3007031.77                | -3005670.77                             | -3007291.96                | -3005932.27                             | 873.13                                  | 877.53                                  |
| 17  | -3407952.70                | -3406606.45                             | -3408246.62                | -3406903.71                             | 986.31                                  | 997.53                                  |
| 18  | -3608408.01                | -3607064.88                             | -3608720.92                | -3607383.09                             | 1050.02                                 | 1067.83                                 |
| 19  | -3808912.37                | -3807561.67                             | -3809230.70                | -3807878.97                             | 1068.21                                 | 1064.77                                 |
| 20  | -4009398.93                | -4008048.56                             | -4009731.19                | -4008379.36                             | 1114.99                                 | 1110.07                                 |
| 30  | -6014058.11                | -6012749.84                             | -6014542.64                | -6013224.01                             | 1625.93                                 | 1591.18                                 |
| 35  | -7016491.74                | -7015179.58                             | -7017022.87                | -7015708.23                             | 1782.33                                 | 1773.99                                 |
| 42  | -7244289.09                | -7242948.86                             | -7244976.80                | -7243637.70                             | 2307.77                                 | 2311.55                                 |
| 54  | -10825497.42               | -10824206.69                            | -10826269.33               | -10824974.92                            | 2590.32                                 | 2577.96                                 |
| 80  | -16037874.76               | -16036561.62                            | -16038966.04               | -16037650.01                            | 3662.00                                 | 3652.34                                 |
| 100 | -20047542.28               | -20046236.30                            | -20048855.98               | -20047547.05                            | 4408.37                                 | 4398.51                                 |

Table S6: Optimized geometries in Cartesian coordinates calculated at the B3LYP/6-31+G(2d,p) level of theory.

| Species                         | Geometry (Å) |          |          |          | Frequencies (cm <sup>-1</sup> ) |           |           |
|---------------------------------|--------------|----------|----------|----------|---------------------------------|-----------|-----------|
| H <sub>2</sub> O                | O            | 0.00000  | 0.00000  | 0.11693  | 1635.1279                       | 3810.0357 | 3922.2869 |
|                                 | H            | 0.00000  | 0.76585  | -0.46772 |                                 |           |           |
|                                 | H            | 0.00000  | -0.76585 | -0.46772 |                                 |           |           |
| (H <sub>2</sub> O) <sub>2</sub> | O            | -0.03491 | 1.56300  | 0.00000  | 190.4568                        | 98.8276   | 123.5913  |
|                                 | H            | 0.09153  | 0.60178  | 0.00000  | 162.5236                        | 368.1293  | 451.3266  |
|                                 | H            | 0.85040  | 1.94007  | 0.00000  | 1633.5572                       | 1661.7016 | 3735.0637 |
|                                 | O            | -0.03491 | -1.39329 | 0.00000  | 3815.1737                       | 3898.2965 | 3927.4065 |
|                                 | H            | 0.55003  | -2.15823 | 0.00000  |                                 |           |           |
|                                 | H            | -0.93338 | -1.74133 | 0.00000  |                                 |           |           |
| (H <sub>2</sub> O) <sub>3</sub> | O            | 0.16529  | 1.60439  | 0.11464  | 176.3851                        | 182.7945  | 206.2712  |
|                                 | H            | 0.12824  | 2.19674  | -0.64387 | 216.5225                        | 219.9481  | 265.7673  |
|                                 | H            | -0.63323 | 1.04132  | 0.05944  | 359.1578                        | 380.0448  | 463.5967  |
|                                 | O            | 1.31342  | -0.94319 | -0.09539 | 603.4234                        | 695.6507  | 927.4207  |
|                                 | H            | 1.92745  | -1.21262 | 0.59528  | 1648.2761                       | 1652.31   | 1673.7017 |
|                                 | H            | 1.21848  | 0.02786  | -0.01797 | 3529.0383                       | 3594.5233 | 3608.3999 |
|                                 | O            | -1.48191 | -0.65310 | -0.09001 | 3878.7602                       | 3883.696  | 3885.1448 |
|                                 | H            | -0.60789 | -1.08945 | -0.05069 |                                 |           |           |
|                                 | H            | -2.00741 | -1.02866 | 0.62389  |                                 |           |           |
| (H <sub>2</sub> O) <sub>4</sub> | O            | -0.62743 | -1.83412 | 0.02114  | 54.511                          | 95.437    | 204.1652  |
|                                 | H            | 0.30874  | -1.52196 | 0.01171  | 236.3697                        | 241.0481  | 241.0599  |
|                                 | H            | -0.72858 | -2.40369 | -0.74872 | 260.7662                        | 283.6801  | 283.7815  |

|                                 |   |          |          |          |           |           |           |
|---------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                 | O | 1.83408  | -0.62749 | -0.02103 | 324.3034  | 429.402   | 462.2405  |
|                                 | H | 2.40415  | -0.72832 | 0.74851  | 477.9532  | 478.0463  | 786.3139  |
|                                 | H | 1.52163  | 0.30860  | -0.01155 | 865.9525  | 865.9682  | 1051.8642 |
|                                 | O | 0.62748  | 1.83412  | 0.02088  | 1653.5783 | 1667.8358 | 1667.877  |
|                                 | H | 0.72890  | 2.40363  | -0.74900 | 1700.5632 | 3318.5409 | 3424.1219 |
|                                 | H | -0.30868 | 1.52200  | 0.01109  | 3424.2132 | 3465.8549 | 3874.9351 |
|                                 | O | -1.83414 | 0.62745  | -0.02092 | 3875.7186 | 3875.7232 | 3877.0096 |
|                                 | H | -2.40400 | 0.72869  | 0.74871  |           |           |           |
|                                 | H | -1.52209 | -0.30874 | -0.01127 |           |           |           |
| (H <sub>2</sub> O) <sub>5</sub> | O | -2.11103 | 0.94037  | -0.08205 | 25.2571   | 44.5004   | 74.9238   |
|                                 | O | 0.24605  | 2.29905  | -0.02189 | 78.0634   | 174.5268  | 222.19    |
|                                 | O | 2.26332  | 0.48026  | 0.10415  | 227.1547  | 234.4811  | 234.7457  |
|                                 | O | 1.15858  | -1.99528 | -0.09490 | 264.3897  | 295.0523  | 301.3485  |
|                                 | O | -1.54628 | -1.73315 | 0.02782  | 303.7491  | 334.4491  | 433.3166  |
|                                 | H | -2.69220 | 1.35611  | 0.56281  | 454.6965  | 481.3043  | 492.5479  |
|                                 | H | 0.41416  | 2.82557  | -0.81056 | 548.8038  | 748.2168  | 827.0623  |
|                                 | H | 2.79294  | 0.48531  | 0.90822  | 907.4645  | 927.711   | 1040.9347 |
|                                 | H | 1.35444  | -2.46497 | -0.91242 | 1655.822  | 1666.6685 | 1677.9632 |
|                                 | H | -1.94682 | -2.11086 | 0.81750  | 1698.735  | 1708.8869 | 3264.147  |
|                                 | H | -1.26720 | 1.45589  | -0.06213 | 3359.0468 | 3368.3355 | 3418.3741 |
|                                 | H | 0.99901  | 1.66080  | 0.04158  | 3428.9047 | 3873.7506 | 3874.9963 |
|                                 | H | 1.89151  | -0.43310 | 0.02660  | 3876.9037 | 3878.5227 | 3880.6735 |
|                                 | H | 0.17316  | -1.92507 | -0.05048 |           |           |           |
|                                 | H | -1.80410 | -0.77967 | 0.01383  |           |           |           |
|                                 |   |          |          |          |           |           |           |

|                                 |   |          |          |          |           |           |           |
|---------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
| (H <sub>2</sub> O) <sub>6</sub> | O | 0.72826  | 0.57445  | -1.61316 | 23.9994   | 32.8335   | 39.6847   |
|                                 | O | -0.62534 | 1.70470  | 0.39846  | 48.9433   | 54.1759   | 84.8301   |
|                                 | O | -2.83676 | 0.08851  | 0.06664  | 161.5937  | 201.5717  | 208.88    |
|                                 | O | -0.85928 | -1.67817 | -0.58376 | 210.2861  | 219.5104  | 233.8778  |
|                                 | O | 2.91671  | 0.02722  | 0.04231  | 238.4072  | 285.4833  | 294.1956  |
|                                 | O | 0.75573  | -0.63676 | 1.64680  | 297.9788  | 310.1892  | 321.0667  |
|                                 | H | 0.26247  | -0.27845 | -1.57038 | 428.6072  | 430.6913  | 457.7434  |
|                                 | H | 1.60904  | 0.39349  | -1.22180 | 476.5713  | 552.0174  | 564.1254  |
|                                 | H | 0.32740  | 0.23246  | 1.57436  | 786.9693  | 807.7569  | 825.0475  |
|                                 | H | 0.24724  | -1.19547 | 1.03265  | 845.4363  | 958.7977  | 987.4494  |
|                                 | H | 2.29162  | -0.29719 | 0.72974  | 1659.1286 | 1669.0031 | 1677.2707 |
|                                 | H | 3.61143  | -0.63368 | -0.03901 | 1695.8398 | 1701.8111 | 1716.0393 |
|                                 | H | -1.69005 | -1.18193 | -0.38929 | 3268.2695 | 3339.18   | 3360.1363 |
|                                 | H | -1.11806 | -2.53646 | -0.93483 | 3408.3931 | 3420.4002 | 3433.6773 |
|                                 | H | -3.30974 | -0.03650 | 0.89640  | 3874.2434 | 3874.3581 | 3878.9923 |
|                                 | H | -2.18727 | 0.80942  | 0.22782  | 3879.3947 | 3883.2661 | 3883.4247 |
|                                 | H | -0.09824 | 1.41894  | -0.40095 |           |           |           |
|                                 | H | -0.58043 | 2.66580  | 0.43701  |           |           |           |
| (H <sub>2</sub> O) <sub>7</sub> | O | -0.95452 | -1.51856 | -1.12775 | 56.2598   | 63.648    | 75.5109   |
|                                 | O | 1.10270  | -0.04542 | -1.88492 | 83.2429   | 85.7951   | 99.9455   |
|                                 | O | 1.07051  | 2.07482  | -0.08549 | 134.9044  | 146.3334  | 178.3818  |
|                                 | O | -2.85321 | 0.39242  | -0.48455 | 180.4315  | 202.6716  | 232.066   |
|                                 | O | -1.12302 | 1.07188  | 1.52088  | 240.298   | 250.8731  | 254.4581  |
|                                 | O | 2.51852  | -0.48221 | 0.54563  | 279.017   | 288.4961  | 297.0684  |
|                                 | O | 0.21009  | -1.52706 | 1.54367  | 313.2855  | 382.8633  | 428.0371  |

|                                 |   |          |          |          |           |           |           |
|---------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                 | H | -0.67072 | -1.76367 | -0.22890 | 437.8193  | 471.7445  | 501.4158  |
|                                 | H | -1.72944 | -0.92809 | -0.99102 | 537.73    | 545.8495  | 584.1252  |
|                                 | H | -3.74183 | 0.20035  | -0.16861 | 616.4793  | 674.3148  | 714.7598  |
|                                 | H | -2.33863 | 0.71637  | 0.29481  | 753.9329  | 793.4173  | 851.6812  |
|                                 | H | -0.41266 | 1.54310  | 1.04653  | 925.0497  | 972.9253  | 1087.5668 |
|                                 | H | -0.73514 | 0.20544  | 1.73872  | 1649.931  | 1660.7966 | 1668.3302 |
|                                 | H | 0.32148  | -2.19347 | 2.22975  | 1678.1236 | 1704.873  | 1711.909  |
|                                 | H | 1.11640  | -1.22746 | 1.28057  | 1729.4914 | 3066.3404 | 3339.6053 |
|                                 | H | 2.26815  | -0.49640 | -0.39821 | 3361.3388 | 3486.5397 | 3519.9173 |
|                                 | H | 2.47448  | 0.45974  | 0.76659  | 3624.7891 | 3629.6675 | 3669.6505 |
|                                 | H | 1.07764  | 2.98935  | -0.38703 | 3696.5422 | 3797.9875 | 3875.973  |
|                                 | H | 1.00977  | 1.51102  | -0.88583 | 3877.4987 | 3879.8659 | 3881.2697 |
|                                 | H | 0.29296  | -0.60831 | -1.69411 |           |           |           |
|                                 | H | 1.29893  | -0.13495 | -2.82299 |           |           |           |
| (H <sub>2</sub> O) <sub>8</sub> | O | 1.41457  | -1.52309 | -1.31886 | 76.8228   | 82.3151   | 82.5136   |
|                                 | O | 1.38662  | -1.40911 | 1.35834  | 82.8838   | 89.6527   | 122.5928  |
|                                 | O | -1.47508 | -1.27923 | 1.50098  | 148.654   | 151.4566  | 152.5504  |
|                                 | O | -1.36551 | 1.39732  | 1.39325  | 164.8183  | 182.2704  | 194.966   |
|                                 | O | 1.50395  | 1.46045  | 1.29667  | 198.7181  | 199.0018  | 270.826   |
|                                 | O | 1.42687  | 1.35038  | -1.38097 | 271.0261  | 282.4015  | 282.6772  |
|                                 | O | -1.44085 | 1.34072  | -1.47913 | 283.2251  | 309.4953  | 310.2651  |
|                                 | O | -1.45035 | -1.33749 | -1.37084 | 327.5409  | 452.8873  | 460.1429  |
|                                 | H | 2.00776  | -2.18758 | -1.68458 | 489.5277  | 490.3221  | 519.177   |
|                                 | H | 1.48983  | -1.57364 | -0.32590 | 566.1831  | 566.9757  | 575.0839  |
|                                 | H | -2.04793 | 1.71728  | -2.12476 | 628.4921  | 663.4094  | 691.924   |

|                                 |   |          |          |          |           |           |           |
|---------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                 | H | -1.53309 | 0.34929  | -1.52991 | 693.3082  | 760.1215  | 760.6254  |
|                                 | H | -1.52164 | -0.28482 | 1.55397  | 781.1583  | 861.3286  | 994.9114  |
|                                 | H | -2.08651 | -1.62946 | 2.15724  | 995.3315  | 1070.0569 | 1093.9437 |
|                                 | H | 0.48105  | 1.49552  | -1.57539 | 1652.9083 | 1658.0639 | 1658.2447 |
|                                 | H | 1.56759  | 0.39904  | -1.54729 | 1674.7902 | 1702.6529 | 1710.9231 |
|                                 | H | -1.61089 | -1.50200 | -0.42245 | 1711.0415 | 1736.3994 | 3172.3287 |
|                                 | H | -0.50895 | -1.56127 | -1.50133 | 3198.6526 | 3228.3802 | 3230.1651 |
|                                 | H | 0.43873  | -1.51254 | 1.56855  | 3596.4726 | 3599.6753 | 3600.7642 |
|                                 | H | 1.57226  | -0.46511 | 1.52256  | 3610.564  | 3633.8265 | 3661.1215 |
|                                 | H | 2.13091  | 2.09763  | 1.65456  | 3662.2561 | 3678.5096 | 3874.6012 |
|                                 | H | 1.56567  | 1.51031  | 0.30276  | 3874.6788 | 3874.7076 | 3875.0365 |
|                                 | H | -0.41328 | 1.57937  | 1.50930  |           |           |           |
|                                 | H | -1.53319 | 1.56848  | 0.44721  |           |           |           |
| (H <sub>2</sub> O) <sub>9</sub> | O | 0.40871  | -1.16462 | 2.10586  | 52.6519   | 66.4057   | 67.2833   |
|                                 | O | 0.37689  | 1.50203  | 1.82997  | 75.7441   | 83.4816   | 83.6764   |
|                                 | O | 2.48476  | 1.35561  | -0.10185 | 87.46     | 121.132   | 149.9836  |
|                                 | O | 2.44508  | -1.31272 | 0.09364  | 153.0027  | 159.4677  | 160.5683  |
|                                 | O | 0.41717  | -1.50162 | -1.92051 | 177.5686  | 190.9363  | 193.794   |
|                                 | O | 0.35194  | 1.17835  | -2.00655 | 201.7046  | 264.5176  | 269.7555  |
|                                 | O | -1.65656 | 1.99510  | -0.12390 | 275.9311  | 279.1586  | 285.6142  |
|                                 | O | -3.32023 | -0.09146 | -0.07389 | 287.6627  | 292.8135  | 314.0835  |
|                                 | O | -1.49050 | -2.03886 | 0.14384  | 321.2008  | 345.631   | 459.1154  |
|                                 | H | 1.88252  | -1.55982 | -0.66522 | 459.2488  | 469.9165  | 505.7197  |
|                                 | H | 1.87075  | -1.43436 | 0.87377  | 526.5955  | 533.9996  | 550.6396  |
|                                 | H | -0.91195 | -1.98040 | -0.64083 | 557.1195  | 605.7535  | 631.6162  |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.90516 | -1.83203 | 0.89735  | 685.1523  | 706.2843  | 718.2594  |
|                                  | H | -0.39568 | 1.50415  | -1.46849 | 745.3446  | 758.5159  | 786.4534  |
|                                  | H | 1.14830  | 1.40265  | -1.48894 | 867.0673  | 914.4045  | 957.9223  |
|                                  | H | 1.16775  | 1.63538  | 1.27347  | 997.7933  | 1058.4974 | 1104.2356 |
|                                  | H | -0.37517 | 1.75865  | 1.26187  | 1657.9109 | 1658.9626 | 1667.9424 |
|                                  | H | 0.35318  | -0.16896 | 2.09575  | 1673.8887 | 1686.4764 | 1691.7686 |
|                                  | H | 0.44477  | -1.43807 | 3.02843  | 1708.2671 | 1727.7317 | 1741.9065 |
|                                  | H | 0.34554  | -0.51532 | -2.04749 | 3157.3897 | 3178.951  | 3192.6063 |
|                                  | H | 0.42832  | -1.90048 | -2.79690 | 3251.7331 | 3281.6086 | 3581.639  |
|                                  | H | 2.60263  | 0.36762  | -0.03086 | 3588.3377 | 3603.641  | 3608.1371 |
|                                  | H | 3.36273  | 1.74878  | -0.14096 | 3620.9355 | 3622.4658 | 3671.4444 |
|                                  | H | -2.34794 | 1.27977  | -0.07952 | 3672.0138 | 3873.3549 | 3874.3064 |
|                                  | H | -2.12173 | 2.82669  | -0.26333 | 3874.4606 | 3876.1472 | 3878.9648 |
|                                  | H | -3.99314 | -0.20807 | 0.60438  |           |           |           |
|                                  | H | -2.69367 | -0.86070 | 0.01471  |           |           |           |
| (H <sub>2</sub> O) <sub>10</sub> | O | 1.69898  | -1.20693 | 1.82661  | 65.8907   | 69.6679   | 72.5043   |
|                                  | H | 1.76234  | -0.21225 | 1.76599  | 73.6659   | 77.248    | 79.8691   |
|                                  | H | 2.27114  | -1.48510 | 2.54939  | 81.6027   | 110.9118  | 115.9919  |
|                                  | O | 1.99640  | -1.58009 | -1.02183 | 141.4504  | 145.9964  | 150.887   |
|                                  | H | 2.03469  | -1.63231 | -0.04885 | 154.614   | 165.4537  | 169.4547  |
|                                  | H | 1.09752  | -1.89032 | -1.25282 | 189.1173  | 199.8365  | 202.59    |
|                                  | O | 1.82041  | 1.42453  | 1.40343  | 229.2082  | 239.0545  | 254.8212  |
|                                  | H | 2.08358  | 1.45084  | 0.46233  | 285.5582  | 292.4033  | 302.3023  |
|                                  | H | 0.92725  | 1.81744  | 1.42528  | 308.7055  | 315.7781  | 323.3969  |
|                                  | O | -0.45617 | 2.07126  | -1.76924 | 324.3375  | 346.944   | 444.6061  |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | 0.46999  | 1.76332  | -1.77765 | 464.1018  | 490.4449  | 503.4807  |
|                                  | H | -0.59800 | 2.39705  | -0.86432 | 513.6777  | 539.4844  | 558.3932  |
|                                  | O | -2.50138 | 0.20817  | 1.22509  | 561.2002  | 578.2227  | 589.5726  |
|                                  | H | -3.29981 | 0.12067  | 1.75639  | 637.372   | 648.8243  | 686.0435  |
|                                  | H | -1.94769 | -0.61081 | 1.39689  | 715.8632  | 719.1051  | 731.5592  |
|                                  | O | 2.20030  | 1.05601  | -1.39394 | 772.5096  | 798.1146  | 822.0812  |
|                                  | H | 2.15951  | 0.05947  | -1.35258 | 841.1863  | 911.5405  | 992.3706  |
|                                  | H | 2.95550  | 1.28634  | -1.94512 | 1064.9077 | 1087.9124 | 1136.0153 |
|                                  | O | -0.85941 | 2.40546  | 1.12892  | 1655.9674 | 1662.9815 | 1664.4718 |
|                                  | H | -1.50784 | 1.67474  | 1.26551  | 1672.7329 | 1675.3705 | 1685.1775 |
|                                  | H | -1.19501 | 3.17426  | 1.60184  | 1695.5296 | 1721.8376 | 1737.3684 |
|                                  | O | -1.00299 | -1.95790 | 1.47608  | 1743.4186 | 3063.1112 | 3107.7195 |
|                                  | H | -0.08324 | -1.74116 | 1.73041  | 3155.4095 | 3211.4498 | 3402.5383 |
|                                  | H | -0.93911 | -2.27962 | 0.55524  | 3429.6168 | 3559.5447 | 3568.1717 |
|                                  | O | -2.15276 | -0.11459 | -1.68534 | 3581.9597 | 3609.1986 | 3617.0565 |
|                                  | H | -1.56323 | 0.66180  | -1.83899 | 3640.0918 | 3664.6306 | 3702.3876 |
|                                  | H | -2.51471 | 0.03190  | -0.79486 | 3720.0575 | 3871.4258 | 3873.5386 |
|                                  | O | -0.72078 | -2.31284 | -1.33600 | 3874.3886 | 3874.6226 | 3876.4749 |
|                                  | H | -1.26624 | -1.50232 | -1.56211 |           |           |           |
|                                  | H | -1.02750 | -3.02868 | -1.90232 |           |           |           |
| (H <sub>2</sub> O) <sub>11</sub> | O | -2.49704 | 1.06124  | 1.72896  | 37.7079   | 42.1379   | 42.7528   |
|                                  | O | -3.26586 | -1.28064 | 0.62745  | 47.887    | 70.6111   | 74.3602   |
|                                  | O | -0.54023 | -2.15504 | 0.89590  | 77.0075   | 83.7386   | 93.0367   |
|                                  | O | 0.29699  | -1.18344 | -1.50977 | 98.3218   | 110.1435  | 121.1173  |
|                                  | O | 0.58791  | 1.38337  | -0.66062 | 128.4788  | 153.712   | 159.4483  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 3.20363  | 2.06378  | -0.30630 | 167.5709  | 174.0823  | 192.4546  |
| O | 3.30815  | -0.15949 | 1.25246  | 195.1958  | 201.5751  | 226.2294  |
| O | 0.38365  | 0.34267  | 1.91912  | 236.1114  | 247.9615  | 259.7468  |
| O | -2.10595 | 2.10424  | -0.93654 | 262.3518  | 271.9068  | 279.6677  |
| O | -2.48872 | -0.34033 | -1.96159 | 291.4517  | 302.4747  | 311.941   |
| O | 3.02858  | -1.84292 | -1.05975 | 322.0267  | 341.767   | 402.6956  |
| H | -2.39220 | 1.60677  | 0.92665  | 430.5082  | 437.1059  | 457.0556  |
| H | -2.31933 | 1.25045  | -1.40622 | 477.1081  | 494.4436  | 509.8857  |
| H | -2.85936 | -0.81018 | -1.18928 | 519.2838  | 532.5496  | 568.7052  |
| H | -3.08408 | -0.43251 | 1.11214  | 583.5614  | 606.8385  | 630.3166  |
| H | 0.48150  | 0.78028  | 1.04362  | 638.5499  | 662.6902  | 693.7191  |
| H | 0.48746  | 0.48558  | -1.07178 | 716.1138  | 740.4037  | 749.1102  |
| H | -0.00572 | -1.62025 | -0.67278 | 786.4818  | 807.9799  | 832.7272  |
| H | -0.23743 | -1.37659 | 1.40573  | 888.3733  | 919.96    | 941.812   |
| H | 3.38909  | 0.67944  | 0.73172  | 970.6488  | 1069.7721 | 1105.3332 |
| H | 3.69991  | 2.02364  | -1.13104 | 1650.6892 | 1654.3572 | 1657.587  |
| H | 3.15441  | -1.37342 | -0.20978 | 1671.233  | 1676.8463 | 1686.2744 |
| H | -1.60035 | 0.94067  | 2.08370  | 1695.7227 | 1712.2006 | 1725.2516 |
| H | -1.60745 | -0.72776 | -2.10358 | 1728.6884 | 1747.0981 | 3192.2683 |
| H | -0.24327 | 1.86132  | -0.84710 | 3237.5845 | 3279.8439 | 3319.494  |
| H | -1.51207 | -2.09698 | 0.90251  | 3347.7139 | 3442.5252 | 3487.4933 |
| H | 1.29848  | 0.18378  | 2.19745  | 3552.5135 | 3576.2445 | 3599.0762 |
| H | 1.22343  | -1.48110 | -1.60656 | 3603.3019 | 3608.4772 | 3632.1894 |
| H | 4.10413  | -0.21973 | 1.79193  | 3681.3377 | 3712.7401 | 3735.4476 |
| H | 3.15226  | -2.77817 | -0.86462 | 3775.993  | 3868.3161 | 3871.4399 |
| H | 2.25562  | 1.96553  | -0.55411 | 3874.4967 | 3874.5773 | 3876.4571 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -2.56577 | 2.81108  | -1.40151 |           |           |           |
|                                  | H | -4.10809 | -1.61938 | 0.94835  |           |           |           |
| (H <sub>2</sub> O) <sub>12</sub> | O | 2.89162  | -1.37298 | -1.45383 | 56.7574   | 58.3664   | 58.3739   |
|                                  | O | 2.84307  | -1.50001 | 1.23816  | 76.7903   | 76.793    | 87.6495   |
|                                  | O | 0.04231  | -1.23615 | -1.52175 | 92.1629   | 92.4767   | 107.773   |
|                                  | O | -0.04188 | 1.52096  | -1.23667 | 113.7495  | 117.5091  | 125.0452  |
|                                  | O | 0.04171  | 1.23582  | 1.52027  | 125.0571  | 152.9418  | 160.1976  |
|                                  | O | -0.04190 | -1.52117 | 1.23520  | 164.728   | 165.7972  | 165.8664  |
|                                  | O | 2.89103  | 1.37332  | 1.45475  | 195.7412  | 201.2284  | 204.7574  |
|                                  | O | 2.84345  | 1.50018  | -1.23733 | 204.779   | 229.2629  | 251.943   |
|                                  | O | -2.89160 | 1.45438  | -1.37276 | 251.978   | 256.3732  | 261.0698  |
|                                  | O | -2.84329 | -1.23777 | -1.49971 | 264.555   | 274.9483  | 274.9688  |
|                                  | O | -2.89107 | -1.45430 | 1.37335  | 301.0685  | 316.2836  | 321.2118  |
|                                  | O | -2.84340 | 1.23766  | 1.50028  | 321.2187  | 443.3408  | 463.8255  |
|                                  | H | 0.04754  | -0.25043 | -1.52892 | 464.8422  | 464.9237  | 504.3677  |
|                                  | H | 0.95414  | -1.49527 | -1.74897 | 514.106   | 523.0372  | 523.0576  |
|                                  | H | 1.92232  | -1.71013 | 1.47485  | 527.1589  | 548.0506  | 573.0339  |
|                                  | H | 2.96186  | -0.56342 | 1.48770  | 573.0937  | 589.1137  | 652.237   |
|                                  | H | 0.04741  | 0.25008  | 1.52727  | 677.106   | 680.9931  | 683.0675  |
|                                  | H | 0.95316  | 1.49540  | 1.74848  | 683.2131  | 721.6319  | 721.7658  |
|                                  | H | 2.96170  | 0.56348  | -1.48676 | 731.8783  | 746.3684  | 746.4989  |
|                                  | H | 1.92306  | 1.71100  | -1.47476 | 841.6242  | 867.2318  | 867.2881  |
|                                  | H | 2.94576  | -1.51376 | -0.46956 | 889.1498  | 998.4665  | 998.5907  |
|                                  | H | 3.57622  | -1.91812 | -1.85599 | 1059.2305 | 1079.8266 | 1102.8999 |
|                                  | H | -0.04740 | -1.52841 | 0.24946  | 1657.1614 | 1657.1759 | 1660.3992 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.04758 | 1.52808  | -0.25094 | 1663.8699 | 1679.2335 | 1679.2478 |
|                                  | H | 2.94547  | 1.51405  | 0.47050  | 1679.4173 | 1697.5017 | 1718.4974 |
|                                  | H | 3.57528  | 1.91877  | 1.85708  | 1724.5831 | 1724.6093 | 1746.5127 |
|                                  | H | -1.92280 | 1.47461  | 1.71076  | 3210.2129 | 3212.355  | 3252.8428 |
|                                  | H | -2.96176 | 1.48695  | 0.56356  | 3252.9398 | 3335.2786 | 3435.4719 |
|                                  | H | -2.94558 | -0.47006 | 1.51416  | 3435.6226 | 3478.9402 | 3604.0715 |
|                                  | H | -2.96114 | -1.48727 | -0.56298 | 3606.1966 | 3608.8216 | 3608.9861 |
|                                  | H | -1.92299 | -1.47511 | -1.71093 | 3654.0198 | 3655.3857 | 3655.6255 |
|                                  | H | -2.94572 | 0.47013  | -1.51351 | 3657.7531 | 3703.4058 | 3703.464  |
|                                  | H | -0.95329 | 1.74921  | -1.49626 | 3703.7439 | 3710.3671 | 3872.3755 |
|                                  | H | -0.95352 | -1.74879 | 1.49471  | 3872.3779 | 3872.5872 | 3872.7379 |
|                                  | H | -3.57695 | 1.85637  | -1.91709 |           |           |           |
|                                  | H | -3.57553 | -1.85676 | 1.91845  |           |           |           |
| (H <sub>2</sub> O) <sub>13</sub> | O | 3.11298  | -1.21376 | 1.87920  | 19.6167   | 27.6054   | 35.9066   |
|                                  | O | 2.54069  | -2.51928 | -0.40236 | 56.7698   | 59.4217   | 60.3845   |
|                                  | O | 0.39033  | -0.31636 | 1.90867  | 67.8649   | 76.6488   | 87.5045   |
|                                  | O | 1.01701  | 1.99355  | 0.51926  | 88.3564   | 94.0772   | 103.9993  |
|                                  | O | -0.18703 | -1.58695 | -0.47991 | 108.8148  | 112.6792  | 120.6236  |
|                                  | O | -2.87486 | -0.80483 | -0.28251 | 124.4274  | 143.2179  | 156.0716  |
|                                  | O | -2.35731 | 0.59570  | 2.02344  | 160.4472  | 164.93    | 171.8409  |
|                                  | O | 0.62062  | 0.66777  | -1.89068 | 186.6071  | 190.3235  | 201.8722  |
|                                  | O | -1.67280 | 2.93456  | 0.45029  | 203.2858  | 223.9245  | 235.3314  |
|                                  | O | -2.15727 | 1.49786  | -1.77082 | 246.4974  | 251.2728  | 254.1787  |
|                                  | O | 3.33681  | -0.24799 | -1.99154 | 258.133   | 264.7214  | 267.3987  |
|                                  | O | 3.76229  | 1.10403  | 0.29908  | 272.1205  | 276.1087  | 278.8236  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | -5.43181 | -2.11794 | -0.31405 | 301.9661  | 314.1425  | 319.3934  |
| H | 0.18524  | -0.86089 | 1.11134  | 450.0403  | 459.6012  | 482.9087  |
| H | 1.24860  | -0.65068 | 2.22610  | 502.6586  | 503.6672  | 509.623   |
| H | 2.97874  | 1.66829  | 0.42455  | 524.4574  | 529.6569  | 556.5225  |
| H | 3.67677  | 0.40020  | 0.97076  | 567.3904  | 598.0029  | 598.3634  |
| H | 0.81807  | 1.21428  | -1.09479 | 615.6837  | 620.6616  | 653.1658  |
| H | 1.49278  | 0.42533  | -2.25063 | 668.9506  | 675.6574  | 682.1299  |
| H | 2.86347  | -1.89743 | -1.08245 | 709.8652  | 730.5392  | 738.6519  |
| H | 1.56990  | -2.49667 | -0.48138 | 746.1408  | 764.5695  | 802.6335  |
| H | 2.95316  | -1.79055 | 1.08259  | 818.5272  | 864.5126  | 875.3873  |
| H | 3.68539  | -1.70829 | 2.47518  | 898.5221  | 972.7485  | 989.5932  |
| H | 0.78283  | 1.23585  | 1.10522  | 1065.4319 | 1077.5162 | 1098.6125 |
| H | 0.05056  | -0.83718 | -1.07254 | 1637.1525 | 1658.2529 | 1659.1868 |
| H | 3.58966  | 0.29683  | -1.19723 | 1662.3769 | 1671.3454 | 1679.4571 |
| H | 4.06373  | -0.18424 | -2.61999 | 1682.4512 | 1693.3807 | 1710.9573 |
| H | -1.28430 | 1.26148  | -2.12917 | 1719.1296 | 1720.663  | 1734.3453 |
| H | -2.51195 | 0.66495  | -1.39554 | 1751.1068 | 3202.8152 | 3203.9128 |
| H | -1.89396 | 2.49444  | -0.41665 | 3247.3374 | 3329.5608 | 3357.3822 |
| H | -2.20110 | 1.48661  | 1.65799  | 3431.456  | 3436.9712 | 3481.0358 |
| H | -1.47785 | 0.27958  | 2.29474  | 3541.4732 | 3591.131  | 3605.0272 |
| H | -2.79485 | -0.36396 | 0.59864  | 3610.3888 | 3621.504  | 3651.5447 |
| H | -1.16522 | -1.60463 | -0.48032 | 3661.1201 | 3664.83   | 3668.777  |
| H | 0.25126  | 2.59506  | 0.56810  | 3692.7574 | 3703.8267 | 3710.4801 |
| H | -3.73234 | -1.26599 | -0.30198 | 3715.8067 | 3803.6857 | 3873.3765 |
| H | -2.10459 | 3.79523  | 0.44814  | 3873.6562 | 3874.5983 | 3911.3976 |
| H | -5.68165 | -2.51650 | 0.52782  |           |           |           |

|                                  |   |          |          |          |          |          |          |
|----------------------------------|---|----------|----------|----------|----------|----------|----------|
|                                  | H | -6.15949 | -1.53205 | -0.55308 |          |          |          |
| (H <sub>2</sub> O) <sub>14</sub> | O | -3.27405 | -0.51125 | 1.96168  | 11.1135  | 22.8093  | 37.4348  |
|                                  | O | -1.70328 | -2.51903 | 1.17770  | 43.0808  | 51.3152  | 65.5999  |
|                                  | O | 0.66154  | -1.34035 | 0.30853  | 69.6113  | 71.6661  | 74.2737  |
|                                  | O | -4.33026 | -0.10785 | -0.65536 | 81.2029  | 83.5008  | 85.9743  |
|                                  | O | -2.73602 | -2.02437 | -1.52888 | 102.3984 | 103.4726 | 109.9778 |
|                                  | O | -0.34109 | -0.90752 | -2.36923 | 131.2507 | 144.117  | 149.354  |
|                                  | O | -2.94765 | 2.35141  | -0.73311 | 149.6982 | 154.1726 | 160.1893 |
|                                  | O | -0.55811 | 1.94478  | -1.84864 | 166.598  | 177.8538 | 188.778  |
|                                  | O | 0.51043  | 1.36944  | 0.68284  | 203.546  | 214.6327 | 226.9342 |
|                                  | O | -1.82908 | 1.95581  | 1.91706  | 232.6083 | 240.1066 | 249.5387 |
|                                  | O | 3.28344  | 1.29223  | 1.43233  | 267.8254 | 279.5786 | 282.691  |
|                                  | O | 4.97667  | 1.42126  | -0.68372 | 284.0039 | 290.0283 | 297.445  |
|                                  | O | 4.93300  | -1.27569 | -0.95150 | 300.5054 | 310.5453 | 321.7838 |
|                                  | O | 3.30860  | -1.63130 | 1.15352  | 326.9331 | 330.5871 | 345.1173 |
|                                  | H | 0.52153  | 0.38514  | 0.59313  | 349.1553 | 446.6995 | 455.7754 |
|                                  | H | 0.30816  | 1.69395  | -0.22029 | 475.1875 | 487.4522 | 493.0393 |
|                                  | H | -1.73483 | 2.56053  | 2.66064  | 503.5565 | 511.4423 | 519.1616 |
|                                  | H | -0.91720 | 1.77472  | 1.56959  | 535.2817 | 548.9369 | 555.4419 |
|                                  | H | 1.52784  | -1.63720 | 0.65211  | 572.0328 | 604.79   | 623.1547 |
|                                  | H | -0.05238 | -1.86597 | 0.72631  | 638.5432 | 657.8059 | 666.7976 |
|                                  | H | -2.27198 | -1.78936 | 1.55562  | 696.4863 | 707.0385 | 716.5323 |
|                                  | H | -1.83798 | -3.29411 | 1.73291  | 726.482  | 756.8171 | 765.5757 |
|                                  | H | -2.77921 | 0.32044  | 2.09304  | 795.3691 | 819.3576 | 832.5795 |
|                                  | H | -3.81420 | -0.35668 | 1.16182  | 877.4227 | 884.1503 | 943.7915 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -3.77026 | -0.83232 | -1.06704 | 955.6893  | 1012.4268 | 1059.0184 |
|                                  | H | -5.23045 | -0.22885 | -0.97514 | 1077.8341 | 1085.1076 | 1131.3036 |
|                                  | H | -2.41782 | -2.41910 | -0.69821 | 1655.3552 | 1656.6826 | 1657.3006 |
|                                  | H | -1.92738 | -1.64298 | -1.94608 | 1664.2412 | 1667.5382 | 1670.069  |
|                                  | H | -0.41618 | 0.06389  | -2.35294 | 1671.9006 | 1681.5877 | 1692.8404 |
|                                  | H | 0.16938  | -1.12632 | -1.56854 | 1694.3285 | 1716.8241 | 1724.9465 |
|                                  | H | -3.50355 | 1.54870  | -0.80846 | 1741.5238 | 1746.2412 | 3065.4562 |
|                                  | H | -2.71076 | 2.40128  | 0.21061  | 3158.938  | 3180.3151 | 3211.7176 |
|                                  | H | -1.48386 | 2.13763  | -1.52822 | 3279.4843 | 3310.8272 | 3377.1362 |
|                                  | H | -0.32479 | 2.63402  | -2.47942 | 3382.7226 | 3419.5968 | 3517.0294 |
|                                  | H | 3.90953  | -1.59723 | 0.36099  | 3537.1201 | 3552.0524 | 3586.707  |
|                                  | H | 3.69379  | -2.26770 | 1.76508  | 3591.0781 | 3604.8829 | 3625.1307 |
|                                  | H | 3.29540  | 0.32726  | 1.56157  | 3632.9599 | 3678.6168 | 3687.729  |
|                                  | H | 2.35735  | 1.49726  | 1.19732  | 3690.3861 | 3695.2892 | 3868.9293 |
|                                  | H | 4.58095  | -1.50116 | -1.81949 | 3872.951  | 3873.2859 | 3873.5822 |
|                                  | H | 5.03606  | -0.29053 | -0.94200 | 3873.682  | 3874.4824 | 3876.5583 |
|                                  | H | 5.79360  | 1.86559  | -0.43418 |           |           |           |
|                                  | H | 4.36612  | 1.49858  | 0.09345  |           |           |           |
| (H <sub>2</sub> O) <sub>15</sub> | O | 3.06950  | -0.36105 | 2.22407  | 53.8675   | 56.113    | 58.8449   |
|                                  | O | 3.02188  | -2.24771 | 0.20318  | 63.9764   | 68.0265   | 73.3175   |
|                                  | O | 2.72289  | -1.00192 | -2.12427 | 74.9056   | 76.6173   | 78.0908   |
|                                  | O | -0.14862 | -1.11894 | -2.01489 | 87.169    | 90.9401   | 93.3321   |
|                                  | O | -0.06494 | 1.59539  | -1.67859 | 103.5326  | 107.9947  | 108.885   |
|                                  | O | -0.10680 | 2.06920  | 1.02019  | 119.3614  | 120.1186  | 136.2698  |
|                                  | O | 0.15092  | -0.32364 | 2.32958  | 142.0308  | 149.4625  | 152.5995  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 0.11222  | -2.31666 | 0.43890  | 159.783   | 165.4498  | 177.4224  |
| O | -2.94394 | 2.09550  | 1.15498  | 181.3233  | 187.7658  | 193.9964  |
| O | -2.96746 | 1.64413  | -1.48967 | 209.134   | 219.362   | 223.8187  |
| O | -2.99415 | -1.15730 | -1.99665 | 233.325   | 247.2597  | 253.7744  |
| O | -2.83200 | -2.38301 | 0.34975  | 279.8856  | 285.9699  | 290.7742  |
| O | -2.80516 | -0.50858 | 2.39570  | 297.4635  | 301.0587  | 307.9821  |
| O | 2.75641  | 2.20004  | 0.92925  | 312.0882  | 317.2182  | 323.7233  |
| O | 2.79471  | 1.81105  | -1.72560 | 332.1626  | 341.6174  | 444.2006  |
| H | 3.16414  | -1.06513 | 1.54045  | 456.8993  | 469.1235  | 476.8915  |
| H | 3.78461  | -0.48623 | 2.85715  | 483.6566  | 496.0535  | 516.2956  |
| H | 2.96707  | -1.78126 | -0.68219 | 528.2656  | 538.9813  | 552.2309  |
| H | 3.67295  | -2.95052 | 0.10182  | 553.8903  | 569.004   | 574.5443  |
| H | 2.84549  | -0.03423 | -2.04299 | 585.713   | 597.8157  | 615.1625  |
| H | 1.78816  | -1.12214 | -2.37143 | 630.9207  | 644.6697  | 654.4778  |
| H | 3.43124  | 2.39061  | -2.15749 | 669.1532  | 673.2365  | 683.8578  |
| H | 2.85640  | 1.98857  | -0.74659 | 693.8904  | 708.6465  | 716.3129  |
| H | 1.82318  | 2.39274  | 1.13392  | 746.8576  | 759.8048  | 780.9154  |
| H | 2.95212  | 1.36619  | 1.39717  | 806.3144  | 812.2157  | 830.4693  |
| H | 1.06882  | -0.36270 | 2.64526  | 861.5195  | 899.0373  | 932.6357  |
| H | 0.07767  | 0.54145  | 1.85723  | 943.8309  | 1013.4524 | 1036.8521 |
| H | 1.03385  | -2.62567 | 0.41945  | 1071.494  | 1089.925  | 1100.8427 |
| H | 0.10052  | -1.60943 | 1.12879  | 1655.721  | 1660.4626 | 1664.3073 |
| H | -0.09512 | -1.55115 | -1.12789 | 1666.5214 | 1673.1425 | 1678.6512 |
| H | -1.07092 | -1.25242 | -2.30460 | 1688.0893 | 1698.632  | 1708.8995 |
| H | 0.82805  | 1.88546  | -1.93672 | 1711.9984 | 1715.6839 | 1722.2496 |
| H | -0.06673 | 0.61535  | -1.80654 | 1735.4572 | 1755.5388 | 1760.9255 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.12270 | 1.89852  | 0.04685  | 3097.9618 | 3106.6941 | 3206.2515 |
|                                  | H | -1.01770 | 2.34209  | 1.23964  | 3212.6466 | 3269.4041 | 3357.257  |
|                                  | H | -1.88023 | -0.51476 | 2.69019  | 3367.4267 | 3416.5144 | 3420.6127 |
|                                  | H | -2.94640 | 0.38575  | 2.03100  | 3424.4187 | 3442.591  | 3560.7209 |
|                                  | H | -1.91879 | -2.70716 | 0.40888  | 3564.0385 | 3607.589  | 3611.7466 |
|                                  | H | -2.91442 | -1.74140 | 1.09482  | 3633.2723 | 3639.7462 | 3664.8868 |
|                                  | H | -3.01104 | -1.63343 | -1.11458 | 3679.6713 | 3689.0752 | 3703.0755 |
|                                  | H | -3.67272 | -1.56463 | -2.54554 | 3712.8437 | 3724.5818 | 3738.7523 |
|                                  | H | -3.08657 | 0.69422  | -1.69474 | 3751.9682 | 3867.3078 | 3870.5294 |
|                                  | H | -2.05808 | 1.84671  | -1.76881 | 3872.3652 | 3872.7834 | 3873.5249 |
|                                  | H | -3.04199 | 1.94290  | 0.17468  |           |           |           |
|                                  | H | -3.61459 | 2.73974  | 1.40534  |           |           |           |
| (H <sub>2</sub> O) <sub>16</sub> | O | -1.47468 | 1.42074  | 1.36157  | 40.0149   | 41.5135   | 43.0093   |
|                                  | H | -2.39376 | 1.63096  | 1.61115  | 62.243    | 65.0771   | 75.8769   |
|                                  | H | -1.45496 | 1.51031  | 0.38089  | 77.4232   | 79.5706   | 82.6143   |
|                                  | O | 1.47460  | -1.41989 | 1.36210  | 90.6712   | 93.7208   | 98.4413   |
|                                  | H | 1.45497  | -1.50994 | 0.38146  | 100.0669  | 103.605   | 107.1805  |
|                                  | H | 2.39362  | -1.63011 | 1.61189  | 107.9943  | 120.7956  | 135.4153  |
|                                  | O | 4.28065  | 1.43838  | 1.30165  | 149.8946  | 151.6229  | 160.2723  |
|                                  | H | 3.35912  | 1.63164  | 1.54977  | 164.6078  | 166.8633  | 173.6396  |
|                                  | H | 4.40593  | 0.49373  | 1.51444  | 184.1648  | 186.0297  | 195.1387  |
|                                  | O | 1.39227  | 1.35427  | 1.42544  | 196.3949  | 196.5876  | 198.1869  |
|                                  | H | 1.37860  | 0.37242  | 1.51236  | 202.2556  | 240.0966  | 246.4909  |
|                                  | H | 0.50810  | 1.64977  | 1.70250  | 248.1806  | 253.92    | 255.5163  |
|                                  | O | 1.39224  | -1.35418 | -1.42524 | 257.4089  | 258.5141  | 265.6257  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | 1.37863  | -0.37232 | -1.51220 | 267.4687  | 277.978   | 278.2383  |
| H | 0.50804  | -1.64963 | -1.70229 | 308.7531  | 313.3966  | 321.7107  |
| O | -4.28054 | 1.43788  | -1.30256 | 322.6849  | 445.2826  | 451.1253  |
| H | -3.35889 | 1.63079  | -1.55054 | 460.5988  | 477.5644  | 495.1521  |
| H | -4.40605 | 0.49320  | -1.51505 | 499.5706  | 503.7393  | 504.9776  |
| O | -4.33059 | -1.44316 | -1.38768 | 517.7164  | 534.2575  | 536.3699  |
| H | -5.00172 | -2.02224 | -1.76430 | 557.303   | 578.1043  | 589.7698  |
| H | -4.39143 | -1.53054 | -0.39720 | 590.9781  | 600.8973  | 606.8894  |
| O | 4.33069  | 1.44227  | -1.38828 | 612.0766  | 614.3786  | 634.9047  |
| H | 4.39124  | 1.53010  | -0.39780 | 650.7723  | 656.0124  | 663.3156  |
| H | 5.00231  | 2.02080  | -1.76488 | 663.4502  | 702.5814  | 709.5258  |
| O | 4.33080  | -1.44239 | 1.38811  | 730.1374  | 736.898   | 741.4165  |
| H | 5.00226  | -2.02095 | 1.76495  | 741.8604  | 764.3117  | 806.6248  |
| H | 4.39148  | -1.53034 | 0.39768  | 827.3518  | 837.2316  | 864.1864  |
| O | -4.28068 | -1.43791 | 1.30229  | 880.7862  | 889.1743  | 906.0605  |
| H | -3.35914 | -1.63101 | 1.55049  | 978.0194  | 982.291   | 1050.1424 |
| H | -4.40599 | -0.49316 | 1.51462  | 1076.1304 | 1076.553  | 1098.5956 |
| O | 1.47467  | 1.41996  | -1.36203 | 1655.1362 | 1656.6799 | 1659.4765 |
| H | 2.39370  | 1.63015  | -1.61185 | 1661.6534 | 1666.0093 | 1677.5465 |
| H | 1.45504  | 1.51014  | -0.38141 | 1685.4918 | 1701.2651 | 1707.6239 |
| O | -1.47462 | -1.42050 | -1.36124 | 1708.3969 | 1710.6894 | 1717.3161 |
| H | -1.45501 | -1.51008 | -0.38056 | 1727.3383 | 1729.329  | 1731.3334 |
| H | -2.39369 | -1.63071 | -1.61092 | 1753.4221 | 3203.0698 | 3203.3537 |
| O | -4.33078 | 1.44289  | 1.38741  | 3244.2229 | 3246.7965 | 3346.755  |
| H | -5.00225 | 2.02177  | 1.76375  | 3347.7003 | 3417.1675 | 3434.3137 |
| H | -4.39128 | 1.53030  | 0.39690  | 3443.4398 | 3472.9871 | 3475.5329 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | O | 4.28055  | -1.43853 | -1.30187 | 3497.4809 | 3606.7404 | 3607.9139 |
|                                  | H | 3.35896  | -1.63167 | -1.54982 | 3610.5596 | 3610.6348 | 3646.9808 |
|                                  | H | 4.40588  | -0.49387 | -1.51460 | 3648.7474 | 3649.4474 | 3653.8801 |
|                                  | O | -1.39225 | 1.35357  | -1.42582 | 3688.2439 | 3692.487  | 3694.5237 |
|                                  | H | -1.37851 | 0.37167  | -1.51232 | 3696.9207 | 3711.0102 | 3713.5248 |
|                                  | H | -0.50816 | 1.64904  | -1.70318 | 3717.2071 | 3724.0269 | 3872.2309 |
|                                  | O | -1.39235 | -1.35339 | 1.42613  | 3872.2482 | 3872.4883 | 3872.566  |
|                                  | H | -0.50819 | -1.64876 | 1.70337  |           |           |           |
|                                  | H | -1.37870 | -0.37150 | 1.51265  |           |           |           |
| (H <sub>2</sub> O) <sub>17</sub> | O | -3.76236 | 2.00454  | -1.38796 | 30.2375   | 36.0731   | 42.9623   |
|                                  | O | -3.99836 | -0.72042 | -1.44469 | 46.3845   | 59.0031   | 66.7958   |
|                                  | O | -3.98596 | -0.84034 | 1.30451  | 69.8547   | 73.8897   | 77.9107   |
|                                  | O | -3.78103 | 1.87806  | 1.56071  | 82.1624   | 82.819    | 89.59     |
|                                  | O | -1.19712 | -1.14156 | -1.39165 | 92.8946   | 98.1061   | 101.8368  |
|                                  | O | 1.65448  | -1.32820 | -1.46347 | 102.5796  | 107.9788  | 114.981   |
|                                  | O | 1.71705  | -1.47838 | 1.31851  | 123.4056  | 132.4093  | 138.6637  |
|                                  | O | 1.90316  | 1.29447  | 1.46003  | 140.8106  | 144.971   | 155.9159  |
|                                  | O | 1.98641  | 1.43144  | -1.32624 | 162.5897  | 168.8634  | 175.7881  |
|                                  | O | -0.93986 | 1.63602  | 1.39546  | 183.4525  | 186.8264  | 189.8184  |
|                                  | O | -0.87935 | 1.62742  | -1.38446 | 195.5303  | 195.885   | 201.0539  |
|                                  | O | -1.13071 | -1.14613 | 1.42100  | 204.9186  | 217.745   | 238.6714  |
|                                  | O | 4.55573  | -1.66668 | 1.44006  | 239.9192  | 245.4662  | 247.4825  |
|                                  | O | 4.77195  | 1.01644  | 1.42844  | 249.7838  | 252.2948  | 255.0705  |
|                                  | O | 4.81193  | 1.08722  | -1.45400 | 255.7973  | 263.4015  | 265.4828  |
|                                  | O | 4.52220  | -1.58847 | -1.44558 | 278.1055  | 296.266   | 309.8956  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | -6.19699 | -2.09109 | -0.18517 | 322.8111  | 334.1035  | 440.2724  |
| H | -2.81462 | 2.12643  | -1.57352 | 449.2051  | 459.6698  | 461.9721  |
| H | 0.02965  | 1.84505  | -1.65359 | 471.4463  | 483.3848  | 495.6303  |
| H | -4.89154 | -1.09554 | -1.50511 | 505.6494  | 506.4519  | 512.3467  |
| H | -2.12590 | -1.25251 | -1.66510 | 518.9118  | 525.4838  | 531.1905  |
| H | 0.74638  | -1.53769 | -1.74260 | 557.2429  | 560.3584  | 583.1645  |
| H | -7.13090 | -2.04651 | 0.04383  | 590.8658  | 602.3634  | 610.5834  |
| H | -4.40352 | 2.29494  | 2.16591  | 640.4456  | 643.599   | 659.11    |
| H | -1.82805 | 1.93081  | 1.66759  | 663.0906  | 676.0356  | 686.2874  |
| H | 1.04798  | 1.66680  | 1.73602  | 689.0322  | 702.4157  | 715.3037  |
| H | -5.70452 | -1.88037 | 0.62498  | 722.7802  | 729.136   | 737.7773  |
| H | -3.14045 | -1.20773 | 1.61800  | 744.8653  | 804.8534  | 832.0949  |
| H | -0.27011 | -1.52577 | 1.66944  | 842.4973  | 852.0168  | 866.9576  |
| H | 1.98421  | 1.49709  | -0.34399 | 886.6823  | 904.8175  | 915.4734  |
| H | 1.69827  | -1.54131 | 0.33578  | 956.7989  | 1005.0182 | 1035.9764 |
| H | 1.72516  | -0.34710 | -1.52270 | 1063.3145 | 1083.4794 | 1102.0374 |
| H | 1.79188  | 0.31690  | 1.51572  | 1644.9617 | 1647.1516 | 1657.1338 |
| H | -0.95672 | 0.65171  | -1.49762 | 1660.6262 | 1662.2897 | 1670.0533 |
| H | -4.05547 | 0.25909  | -1.56334 | 1673.5341 | 1679.1972 | 1685.7972 |
| H | -0.92383 | 1.74466  | 0.41607  | 1690.4478 | 1693.7508 | 1713.1603 |
| H | -3.94572 | 0.90246  | 1.59734  | 1716.7356 | 1724.0487 | 1726.9296 |
| H | -1.20449 | -1.26049 | -0.41555 | 1729.6846 | 1749.8365 | 3203.2972 |
| H | -3.89356 | -0.81972 | 0.32097  | 3244.881  | 3297.9403 | 3353.6392 |
| H | -1.02054 | -0.17195 | 1.51684  | 3358.4287 | 3368.6615 | 3417.7161 |
| H | -3.85270 | 2.16600  | -0.43217 | 3431.1153 | 3439.372  | 3460.9559 |
| H | 2.92052  | 1.54510  | -1.58300 | 3470.8394 | 3488.3642 | 3508.952  |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | 3.58133  | -1.74697 | -1.64086 | 3608.2502 | 3611.7544 | 3643.2283 |
|                                  | H | 2.61510  | -1.76368 | 1.57086  | 3645.3226 | 3648.1832 | 3659.0093 |
|                                  | H | 3.87835  | 1.34872  | 1.62661  | 3664.2115 | 3685.0737 | 3690.6676 |
|                                  | H | 4.77898  | 0.09562  | -1.54407 | 3693.1819 | 3703.6322 | 3708.2384 |
|                                  | H | 4.62519  | -1.80535 | -0.49947 | 3711.4514 | 3714.6014 | 3719.6341 |
|                                  | H | 4.70937  | -0.68643 | 1.52840  | 3727.7707 | 3748.5527 | 3872.7261 |
|                                  | H | 4.91024  | 1.20861  | 0.48129  | 3873.0469 | 3874.3252 | 3894.4366 |
|                                  | H | 5.51755  | 1.40114  | -2.02942 |           |           |           |
|                                  | H | 5.19315  | -2.10667 | 2.01245  |           |           |           |
| (H <sub>2</sub> O) <sub>18</sub> | O | 4.98833  | -1.35184 | 1.39723  | 29.7989   | 32.3293   | 35.2824   |
|                                  | O | 5.02706  | 1.33776  | 1.48779  | 37.7758   | 49.1412   | 57.5247   |
|                                  | O | 2.18347  | 1.42083  | 1.36415  | 65.5911   | 68.7532   | 70.934    |
|                                  | O | 2.10675  | 1.36076  | -1.42201 | 74.7442   | 76.32     | 83.1649   |
|                                  | O | -0.75053 | 1.43584  | -1.34820 | 85.817    | 89.8071   | 92.5427   |
|                                  | O | -3.58890 | 1.35713  | -1.44919 | 98.8103   | 100.3191  | 103.7604  |
|                                  | O | 2.18347  | -1.42082 | -1.36413 | 113.9302  | 121.9776  | 123.7318  |
|                                  | O | 2.10673  | -1.36075 | 1.42202  | 134.6635  | 143.7523  | 151.1419  |
|                                  | O | -0.75054 | -1.43584 | 1.34821  | 158.8277  | 163.6801  | 167.632   |
|                                  | O | -3.58890 | -1.35713 | 1.44919  | 174.5811  | 174.7554  | 177.4688  |
|                                  | O | -0.68351 | 1.35706  | 1.45539  | 183.3225  | 183.7124  | 188.9848  |
|                                  | O | -0.68351 | -1.35705 | -1.45537 | 192.951   | 196.2267  | 198.7427  |
|                                  | O | -5.72266 | -2.72932 | 0.14997  | 201.7536  | 209.9343  | 214.2751  |
|                                  | O | -5.72266 | 2.72932  | -0.15000 | 227.2038  | 227.6436  | 242.4839  |
|                                  | O | -3.57708 | -1.45011 | -1.35093 | 242.954   | 244.0518  | 251.9385  |
|                                  | O | -3.57708 | 1.45011  | 1.35094  | 254.4647  | 256.6596  | 257.4258  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 5.02707  | -1.33779 | -1.48782 | 265.5624  | 278.1788  | 308.3912  |
| O | 4.98831  | 1.35186  | -1.39723 | 321.851   | 336.7786  | 341.8855  |
| H | 4.06714  | -1.60446 | 1.58676  | 445.3017  | 458.6354  | 465.4451  |
| H | 1.21961  | -1.65912 | 1.68781  | 473.6489  | 480.4059  | 488.3247  |
| H | -1.66064 | -1.65791 | 1.61550  | 497.9494  | 498.8904  | 505.6783  |
| H | 5.10942  | -1.52800 | 0.44474  | 506.3754  | 519.8332  | 521.1394  |
| H | 3.10362  | -1.61293 | -1.62472 | 525.9762  | 547.7279  | 557.6538  |
| H | 0.21292  | -1.63478 | -1.71228 | 558.3457  | 582.5815  | 585.4797  |
| H | -2.70033 | -1.68179 | -1.70246 | 603.4086  | 606.1972  | 642.9187  |
| H | 5.10941  | 1.52801  | -0.44473 | 644.4423  | 648.2421  | 663.3852  |
| H | 5.08657  | -0.34511 | -1.54720 | 672.0753  | 681.994   | 685.6019  |
| H | 3.10362  | 1.61291  | 1.62472  | 695.3758  | 714.0624  | 721.2552  |
| H | 0.21292  | 1.63479  | 1.71230  | 732.1602  | 737.5298  | 742.4537  |
| H | -2.70034 | 1.68179  | 1.70246  | 791.0746  | 797.2638  | 825.2843  |
| H | 4.06713  | 1.60449  | -1.58674 | 830.7193  | 858.8553  | 864.96    |
| H | 1.21962  | 1.65911  | -1.68779 | 891.9482  | 895.1042  | 901.2694  |
| H | -1.66064 | 1.65790  | -1.61549 | 924.0143  | 1005.177  | 1030.6873 |
| H | 5.08655  | 0.34506  | 1.54706  | 1056.8606 | 1079.753  | 1099.8226 |
| H | -3.76747 | -0.40429 | 1.59869  | 1637.3023 | 1642.1803 | 1647.8089 |
| H | -3.76746 | 0.40428  | -1.59869 | 1650.4981 | 1657.6066 | 1661.9527 |
| H | -3.44213 | -1.41171 | -0.37803 | 1670.872  | 1678.3895 | 1679.5401 |
| H | -3.44214 | 1.41172  | 0.37804  | 1686.6868 | 1689.9491 | 1696.606  |
| H | -0.74585 | -1.51911 | 0.36758  | 1714.7958 | 1717.2539 | 1724.4946 |
| H | 2.17250  | -1.51452 | -0.38392 | 1727.1017 | 1729.5678 | 1749.6646 |
| H | -0.67896 | 0.37509  | 1.52911  | 3202.4411 | 3244.1144 | 3353.7494 |
| H | 2.17249  | 1.51453  | 0.38394  | 3370.6706 | 3423.1495 | 3433.3275 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.67897 | -0.37508 | -1.52909 | 3439.6385 | 3458.9147 | 3468.8304 |
|                                  | H | 2.08787  | 0.37942  | -1.50872 | 3484.3002 | 3491.831  | 3506.5953 |
|                                  | H | -0.74584 | 1.51912  | -0.36757 | 3527.4229 | 3546.7631 | 3608.6058 |
|                                  | H | 2.08783  | -0.37940 | 1.50865  | 3611.3406 | 3644.2448 | 3645.0823 |
|                                  | H | -4.43879 | -1.83052 | 1.41435  | 3665.5885 | 3666.8077 | 3683.437  |
|                                  | H | -4.43878 | 1.83051  | -1.41436 | 3685.4432 | 3689.9015 | 3694.9993 |
|                                  | H | -5.20434 | -2.57069 | -0.65717 | 3698.1643 | 3699.8357 | 3702.3695 |
|                                  | H | -5.20435 | 2.57070  | 0.65714  | 3707.8543 | 3712.0474 | 3717.5287 |
|                                  | H | 5.70233  | -1.69796 | -2.07248 | 3720.6909 | 3726.4014 | 3872.7442 |
|                                  | H | 5.70235  | 1.69785  | 2.07248  | 3873.0252 | 3890.1919 | 3890.2811 |
|                                  | H | -5.98669 | -3.65490 | 0.12536  |           |           |           |
|                                  | H | -5.98668 | 3.65489  | -0.12540 |           |           |           |
| (H <sub>2</sub> O) <sub>19</sub> | O | 4.95386  | 1.07312  | -1.03103 | 27.0124   | 36.492    | 40.1415   |
|                                  | O | 4.59430  | 0.88421  | 1.64168  | 50.217    | 54.4196   | 59.4693   |
|                                  | O | 2.32124  | 1.38885  | -2.06309 | 67.6947   | 69.2585   | 72.4573   |
|                                  | O | 1.23350  | 2.96339  | -0.23082 | 75.6712   | 76.5189   | 78.6823   |
|                                  | O | 1.72212  | -1.33296 | -1.56533 | 79.4436   | 87.1338   | 89.9776   |
|                                  | O | 1.80563  | -1.40347 | 1.18942  | 90.4439   | 93.645    | 94.9357   |
|                                  | O | -1.22725 | -1.74950 | -1.52724 | 102.5098  | 108.3859  | 115.1506  |
|                                  | O | -1.73610 | 0.72302  | -2.47236 | 123.1111  | 134.6933  | 136.9114  |
|                                  | O | -0.96626 | -1.68066 | 1.20582  | 144.4377  | 151.1218  | 155.7274  |
|                                  | O | -1.26642 | 0.89779  | 2.07419  | 161.6432  | 165.9454  | 167.9486  |
|                                  | O | -1.53668 | 2.38412  | -0.23926 | 171.9564  | 175.6026  | 183.0078  |
|                                  | O | 1.64273  | 1.26916  | 1.96531  | 190.2947  | 192.4743  | 199.7831  |
|                                  | O | -4.02223 | -2.33098 | -1.21716 | 208.4745  | 217.161   | 230.277   |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | -3.75769 | -2.22180 | 1.44752  | 233.1231  | 236.6658  | 247.8062  |
| O | 4.53863  | -1.96299 | 1.35474  | 259.8867  | 266.3145  | 280.574   |
| O | 4.59403  | -1.76690 | -1.31544 | 281.6851  | 289.457   | 292.2826  |
| O | -4.06203 | 0.45847  | 2.42353  | 297.3928  | 300.702   | 309.0277  |
| O | -4.43592 | 1.99787  | 0.29831  | 313.7669  | 315.8985  | 318.9039  |
| O | -4.58662 | 0.40050  | -1.96305 | 333.1874  | 341.1859  | 348.6384  |
| H | 4.84558  | 1.10078  | -0.04305 | 448.4875  | 459.0769  | 465.2804  |
| H | 5.74800  | 1.57520  | -1.24277 | 473.3649  | 480.1609  | 495.3345  |
| H | 4.67431  | -0.08286 | 1.74805  | 500.863   | 504.0237  | 505.1584  |
| H | 3.70734  | 1.11199  | 1.96693  | 513.732   | 526.6269  | 536.1121  |
| H | 5.06127  | -2.67985 | 1.72886  | 541.1092  | 546.1128  | 561.696   |
| H | 4.63496  | -2.00247 | 0.36292  | 585.4691  | 588.5633  | 596.9884  |
| H | 3.67068  | -1.81704 | -1.62303 | 614.3572  | 628.7544  | 635.5971  |
| H | 4.83792  | -0.82598 | -1.40203 | 640.6484  | 650.4802  | 655.6896  |
| H | 3.27261  | 1.36405  | -1.84395 | 660.5825  | 671.1538  | 684.9894  |
| H | 2.02018  | 0.46079  | -1.95870 | 700.819   | 703.0512  | 709.2904  |
| H | 1.64455  | 3.83346  | -0.27450 | 714.8491  | 724.7027  | 740.675   |
| H | 1.63205  | 2.41225  | -0.96746 | 746.7872  | 767.8339  | 794.0673  |
| H | 1.52781  | 1.90617  | 1.22696  | 798.8497  | 829.7269  | 836.9383  |
| H | 0.77154  | 1.24093  | 2.39830  | 860.3168  | 872.7623  | 901.6215  |
| H | 2.68835  | -1.75131 | 1.42238  | 927.7295  | 971.0037  | 986.2569  |
| H | 1.79554  | -0.45783 | 1.46247  | 987.5032  | 1024.9196 | 1043.0003 |
| H | 1.69508  | -1.38108 | -0.58018 | 1071.5513 | 1081.2133 | 1094.7925 |
| H | 0.87176  | -1.69634 | -1.86162 | 1652.0241 | 1654.8971 | 1660.7352 |
| H | -1.20580 | 0.92502  | -3.25092 | 1664.4287 | 1669.3371 | 1675.2449 |
| H | -1.47696 | -0.18699 | -2.16710 | 1685.8594 | 1686.6274 | 1692.9    |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.65755 | 2.80683  | -0.27399 | 1696.5479 | 1703.0778 | 1708.8796 |
|                                  | H | -1.58026 | 1.82916  | -1.04785 | 1713.1998 | 1722.6223 | 1725.8037 |
|                                  | H | -1.39543 | 1.42547  | 1.24983  | 1735.3753 | 1738.4589 | 1753.1881 |
|                                  | H | -2.15482 | 0.84462  | 2.47635  | 1763.9104 | 3095.5585 | 3101.6845 |
|                                  | H | -1.05908 | -0.74862 | 1.52382  | 3193.7482 | 3195.5788 | 3225.506  |
|                                  | H | -0.03523 | -1.90565 | 1.38494  | 3265.9789 | 3317.0817 | 3369.3946 |
|                                  | H | -1.12524 | -1.70162 | -0.54427 | 3386.1462 | 3410.4317 | 3415.5281 |
|                                  | H | -2.10112 | -2.16864 | -1.64624 | 3454.1087 | 3511.2734 | 3515.303  |
|                                  | H | -2.78939 | -2.27382 | 1.54441  | 3524.8768 | 3580.1554 | 3587.6138 |
|                                  | H | -4.68514 | 0.68259  | 3.12294  | 3604.6622 | 3614.1481 | 3623.5797 |
|                                  | H | -3.58395 | 2.43631  | 0.14236  | 3625.2408 | 3628.6575 | 3630.4332 |
|                                  | H | -3.72248 | 0.58590  | -2.36842 | 3639.205  | 3657.2234 | 3683.4764 |
|                                  | H | -4.59279 | -3.06330 | -1.47376 | 3689.8358 | 3703.5944 | 3713.1714 |
|                                  | H | -4.58444 | 1.44111  | -0.50310 | 3734.734  | 3739.0894 | 3740.7705 |
|                                  | H | -4.28290 | 1.04498  | 1.64129  | 3868.0343 | 3868.7452 | 3870.4968 |
|                                  | H | -3.99194 | -1.34703 | 1.81690  | 3871.1226 | 3872.761  | 3876.3589 |
|                                  | H | -4.54237 | -0.54691 | -1.73323 |           |           |           |
|                                  | H | -4.00348 | -2.32014 | -0.21953 |           |           |           |
| (H <sub>2</sub> O) <sub>20</sub> | O | 3.10235  | 2.31145  | -0.78258 | 50.3401   | 50.8357   | 51.6337   |
|                                  | O | 0.58168  | 3.73334  | -0.81053 | 53.1184   | 53.4704   | 57.5793   |
|                                  | O | 2.93931  | 0.27790  | -2.60963 | 59.0782   | 60.5048   | 62.4646   |
|                                  | O | 3.28789  | 1.05209  | 1.78206  | 64.7976   | 66.5519   | 67.6881   |
|                                  | O | -1.02576 | 2.71841  | -2.61720 | 69.056    | 70.4331   | 73.3326   |
|                                  | O | 0.30457  | 0.49766  | -3.80601 | 74.6425   | 75.3553   | 93.2591   |
|                                  | O | -0.55742 | 3.44018  | 1.66526  | 94.768    | 96.8557   | 98.5303   |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | 2.99546  | -2.00590 | -1.31137 | 98.9185  | 101.1425 | 102.9623 |
| O | 1.06640  | 1.77542  | 3.32459  | 122.5778 | 138.859  | 139.9602 |
| O | 3.32573  | -1.56184 | 1.42968  | 141.5982 | 162.4633 | 163.1044 |
| O | -3.23306 | 1.61374  | -1.29957 | 163.537  | 170.4783 | 172.9433 |
| O | -1.12322 | -1.76031 | -3.23036 | 181.1561 | 190.7697 | 195.1005 |
| O | -3.09271 | 2.08586  | 1.26531  | 196.8353 | 201.423  | 205.429  |
| O | 0.58311  | -3.49101 | -1.65777 | 207.7346 | 210.4094 | 240.9677 |
| O | -0.30784 | -0.40847 | 3.82857  | 243.9831 | 249.7464 | 257.5202 |
| O | 0.98413  | -2.57441 | 2.72861  | 262.3831 | 265.1386 | 308.2405 |
| O | -3.25628 | -1.16009 | -1.84438 | 309.0515 | 313.4873 | 325.9337 |
| O | -2.92177 | -0.28519 | 2.58826  | 333.9212 | 337.1883 | 342.0179 |
| O | -0.72075 | -3.78878 | 0.72120  | 343.4294 | 347.5697 | 349.0422 |
| O | -2.92883 | -2.37666 | 0.65360  | 352.7255 | 357.0142 | 361.7022 |
| H | 3.10459  | 1.60709  | -1.47569 | 370.3212 | 374.9745 | 376.2023 |
| H | 3.84951  | 2.88956  | -0.97241 | 385.6287 | 450.7965 | 456.0591 |
| H | 1.43787  | 3.26981  | -0.78698 | 464.3112 | 488.2801 | 501.5975 |
| H | 0.19731  | 3.65502  | 0.09672  | 503.7063 | 510.6489 | 559.616  |
| H | 3.59490  | 0.20440  | -3.31217 | 569.8067 | 574.7793 | 583.7017 |
| H | 2.95903  | -0.59894 | -2.11658 | 588.1281 | 595.6929 | 613.0525 |
| H | 3.21455  | 1.52307  | 0.93038  | 629.1895 | 630.0643 | 634.9746 |
| H | 2.52384  | 1.33690  | 2.32803  | 640.397  | 651.1059 | 656.5568 |
| H | -1.23682 | 3.42408  | -3.23838 | 682.3195 | 692.8524 | 705.6297 |
| H | -0.41172 | 3.12243  | -1.92858 | 708.2874 | 721.1778 | 724.8674 |
| H | -0.13388 | 1.28249  | -3.42155 | 734.6419 | 742.6091 | 746.3495 |
| H | 1.19201  | 0.46120  | -3.40574 | 759.2096 | 761.006  | 770.1748 |
| H | -1.40665 | 2.97325  | 1.56446  | 780.0167 | 807.6957 | 825.8646 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | -0.01531 | 2.88777  | 2.26172  | 832.0089  | 844.0418  | 856.6871  |
| H | 3.13905  | -1.88616 | -0.34822 | 858.6018  | 861.7178  | 879.9783  |
| H | 2.17716  | -2.53077 | -1.40618 | 883.6487  | 904.9683  | 1067.3483 |
| H | 0.54445  | 0.94100  | 3.53252  | 1101.5395 | 1102.8938 | 1117.8453 |
| H | 1.28627  | 2.17447  | 4.17361  | 1145.7801 | 1153.012  | 1165.6294 |
| H | 4.14086  | -1.89306 | 1.82246  | 1659.8034 | 1663.5012 | 1666.0369 |
| H | 3.32379  | -0.56916 | 1.57818  | 1668.4609 | 1670.8816 | 1672.2768 |
| H | -3.24874 | 0.66130  | -1.52619 | 1673.9844 | 1679.9365 | 1682.5407 |
| H | -2.47832 | 2.00548  | -1.78954 | 1685.1171 | 1690.6085 | 1697.8799 |
| H | -0.52483 | -2.34285 | -2.72907 | 1698.8972 | 1702.2054 | 1712.1997 |
| H | -0.59758 | -0.95557 | -3.46498 | 1716.442  | 1728.2249 | 1729.6034 |
| H | -3.80498 | 2.70321  | 1.46589  | 1733.7266 | 1737.937  | 2948.34   |
| H | -3.15060 | 1.90289  | 0.27404  | 2969.1481 | 3017.3108 | 3020.9452 |
| H | 0.71807  | -4.34442 | -2.08446 | 3022.1391 | 3033.8034 | 3098.2663 |
| H | 0.11145  | -3.67096 | -0.80706 | 3337.737  | 3351.0047 | 3362.9592 |
| H | -1.19304 | -0.38111 | 3.42314  | 3374.4648 | 3383.5118 | 3394.9642 |
| H | 0.14059  | -1.20771 | 3.46098  | 3498.4533 | 3503.2554 | 3507.548  |
| H | 1.79527  | -2.26205 | 2.28349  | 3510.2162 | 3560.652  | 3581.8189 |
| H | 0.43919  | -2.99125 | 2.03697  | 3583.8143 | 3589.0271 | 3600.5622 |
| H | -4.01833 | -1.44151 | -2.36262 | 3607.1013 | 3619.4128 | 3657.464  |
| H | -2.44087 | -1.39196 | -2.39224 | 3659.8627 | 3662.5613 | 3668.7784 |
| H | -3.63531 | -0.37072 | 3.23025  | 3671.6449 | 3674.2106 | 3861.9089 |
| H | -3.04146 | 0.59344  | 2.14747  | 3862.2893 | 3862.4247 | 3864.149  |
| H | -0.97234 | -4.66662 | 1.02928  | 3865.0685 | 3865.3189 | 3865.6101 |
| H | -1.56957 | -3.24673 | 0.69789  | 3867.1057 | 3867.4957 | 3868.5927 |
| H | -2.94475 | -1.65299 | 1.31034  |           |           |           |

|                                  |   |          |          |          |          |          |          |
|----------------------------------|---|----------|----------|----------|----------|----------|----------|
|                                  | H | -3.08864 | -1.96122 | -0.22096 |          |          |          |
| (H <sub>2</sub> O) <sub>30</sub> | O | -3.38188 | 1.94674  | 3.52917  | 24.0482  | 31.2579  | 32.8313  |
|                                  | H | -2.92057 | 2.48330  | 2.85207  | 34.869   | 35.81    | 39.5397  |
|                                  | H | -4.30053 | 2.23625  | 3.51969  | 41.3047  | 44.6718  | 45.8875  |
|                                  | O | -3.38073 | -2.44169 | -1.38993 | 48.2215  | 50.6095  | 50.871   |
|                                  | H | -2.44120 | -2.39567 | -1.62742 | 53.1877  | 54.8909  | 56.0913  |
|                                  | H | -3.54810 | -1.63652 | -0.83754 | 60.0018  | 61.2067  | 64.8075  |
|                                  | O | -5.04756 | 1.25812  | -2.20149 | 67.2735  | 70.3428  | 70.7147  |
|                                  | H | -4.27308 | 1.78720  | -1.95515 | 71.7698  | 74.1423  | 75.7704  |
|                                  | H | -5.25680 | 0.77787  | -1.38625 | 78.6201  | 79.5983  | 81.9997  |
|                                  | O | -2.85832 | -0.65818 | 2.64813  | 84.5223  | 87.3836  | 90.9766  |
|                                  | H | -3.33894 | -1.44711 | 2.99689  | 92.6811  | 95.7765  | 97.2675  |
|                                  | H | -3.12014 | 0.15383  | 3.12944  | 98.4438  | 101.6616 | 102.9925 |
|                                  | O | 1.98204  | 4.52710  | 1.57740  | 111.6009 | 114.3647 | 119.9016 |
|                                  | H | 1.60359  | 4.09743  | 2.36379  | 124.2212 | 130.8136 | 131.2159 |
|                                  | H | 1.22014  | 4.94821  | 1.13493  | 136.2988 | 137.3135 | 143.2594 |
|                                  | O | 5.06252  | 1.38562  | -0.62075 | 149.0475 | 150.5461 | 157.7187 |
|                                  | H | 5.30105  | 0.52266  | -0.17373 | 161.2784 | 167.4963 | 169.3468 |
|                                  | H | 5.86139  | 1.92370  | -0.62538 | 174.5151 | 179.0601 | 181.6297 |
|                                  | O | -0.20374 | -3.39503 | 0.34767  | 183.4798 | 189.1222 | 189.9975 |
|                                  | H | -0.34615 | -3.05133 | -0.55373 | 193.4829 | 198.722  | 200.7715 |
|                                  | H | -0.30729 | -2.62722 | 0.96258  | 205.2685 | 208.346  | 213.6261 |
|                                  | O | 2.63346  | -2.07249 | -2.13819 | 215.868  | 217.4905 | 219.1155 |
|                                  | H | 1.74014  | -2.22117 | -2.49023 | 225.5091 | 228.9847 | 232.2487 |
|                                  | H | 2.59707  | -2.45868 | -1.23753 | 235.6554 | 241.2037 | 244.8515 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | -0.37170 | -2.17387 | -2.28435 | 250.9955 | 254.3857 | 258.4826 |
| H | -0.73478 | -2.23279 | -3.18413 | 264.3891 | 267.4464 | 275.5917 |
| H | -0.35503 | -1.19724 | -2.13444 | 280.7332 | 281.9306 | 287.3033 |
| O | 5.63330  | -0.96709 | 0.46660  | 291.0034 | 292.5552 | 296.6002 |
| H | 5.55171  | -1.64659 | -0.23234 | 302.1159 | 309.298  | 311.8422 |
| H | 5.03510  | -1.23377 | 1.19041  | 314.9981 | 319.0333 | 333.2181 |
| O | -2.38434 | 2.01455  | -0.87752 | 342.1805 | 347.4369 | 353.2116 |
| H | -2.02756 | 2.30484  | -0.01227 | 358.9382 | 381.2333 | 424.6886 |
| H | -1.70693 | 1.44627  | -1.31602 | 431.4639 | 434.8386 | 445.2647 |
| O | -1.62800 | 3.12973  | 1.64774  | 450.4671 | 455.3699 | 472.5474 |
| H | -1.42807 | 4.02765  | 1.31633  | 474.0015 | 484.4343 | 488.0746 |
| H | -0.85484 | 2.90142  | 2.20811  | 488.7768 | 493.363  | 501.5409 |
| O | 0.58950  | 2.67253  | 3.31749  | 504.5092 | 513.7931 | 527.3786 |
| H | 0.39686  | 2.58648  | 4.25746  | 540.6012 | 546.1009 | 552.6901 |
| H | 1.04768  | 1.84143  | 3.02944  | 568.2276 | 572.8703 | 574.8572 |
| O | -0.65613 | 4.20066  | -2.06362 | 578.282  | 588.8135 | 591.593  |
| H | 0.11572  | 3.67353  | -2.34340 | 603.7067 | 606.4109 | 611.825  |
| H | -1.36473 | 3.55533  | -1.89843 | 615.3752 | 622.5863 | 629.0344 |
| O | 3.47829  | -1.67135 | 2.32704  | 642.6841 | 646.258  | 657.7572 |
| H | 3.11840  | -2.27264 | 1.64196  | 665.6178 | 672.7052 | 682.9153 |
| H | 2.97667  | -0.83319 | 2.23112  | 684.8769 | 690.9551 | 700.2625 |
| O | -0.60948 | 0.53639  | -2.32550 | 712.0782 | 713.111  | 721.6643 |
| H | 0.19345  | 1.12115  | -2.39433 | 726.5512 | 729.214  | 740.0753 |
| H | -0.95725 | 0.37769  | -3.22831 | 747.3708 | 759.7119 | 762.8973 |
| O | -4.21764 | -0.98692 | -3.75497 | 775.1719 | 779.9903 | 794.7548 |
| H | -4.13161 | -1.62730 | -3.02290 | 798.0349 | 806.5294 | 825.529  |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | -4.54772 | -0.16699 | -3.33117 | 829.4828  | 843.5542  | 846.6     |
| O | 1.42670  | -2.53758 | 4.06448  | 862.0921  | 865.5014  | 875.5804  |
| H | 1.52295  | -2.35970 | 5.00554  | 882.4951  | 882.985   | 900.136   |
| H | 2.27911  | -2.29222 | 3.64489  | 905.5374  | 926.232   | 929.2111  |
| O | 1.45684  | 2.22651  | -2.35047 | 948.023   | 977.3669  | 993.3656  |
| H | 2.19643  | 1.74295  | -2.78974 | 1002.3324 | 1031.942  | 1046.8717 |
| H | 1.77847  | 2.29918  | -1.42111 | 1048.1747 | 1064.364  | 1067.599  |
| O | -3.89420 | -0.21270 | 0.09763  | 1081.3428 | 1097.8057 | 1121.137  |
| H | -3.61082 | -0.38985 | 1.02135  | 1630.6395 | 1633.439  | 1649.5676 |
| H | -3.34991 | 0.54453  | -0.19457 | 1656.7382 | 1658.1283 | 1659.4133 |
| O | 2.55131  | 2.27658  | 0.17293  | 1663.8369 | 1665.4459 | 1667.6866 |
| H | 2.46549  | 3.14652  | 0.63984  | 1669.7369 | 1670.4838 | 1673.6832 |
| H | 3.50000  | 2.10360  | -0.00998 | 1676.2072 | 1682.162  | 1683.261  |
| O | -3.02350 | -4.26559 | 0.82753  | 1686.8305 | 1692.3398 | 1693.2861 |
| H | -3.32717 | -3.77139 | 0.04090  | 1697.7132 | 1703.2058 | 1704.0527 |
| H | -2.05455 | -4.19773 | 0.77985  | 1707.2702 | 1716.4997 | 1717.7806 |
| O | -4.02134 | -3.05185 | 3.06073  | 1726.0481 | 1728.3561 | 1736.9124 |
| H | -3.96499 | -3.65570 | 3.80754  | 1737.9151 | 1738.6899 | 1751.0063 |
| H | -3.67759 | -3.54480 | 2.27290  | 3111.4466 | 3131.6007 | 3185.5648 |
| O | -0.46905 | 5.37451  | 0.34119  | 3222.0326 | 3230.1976 | 3252.837  |
| H | -0.72070 | 6.30242  | 0.27944  | 3284.6287 | 3306.376  | 3314.0466 |
| H | -0.48897 | 5.01114  | -0.58601 | 3341.4661 | 3366.4006 | 3374.0284 |
| O | 3.57709  | 0.57865  | -2.98162 | 3387.6123 | 3407.3133 | 3417.1465 |
| H | 4.20585  | 0.86618  | -2.29394 | 3425.3022 | 3443.4112 | 3456.1819 |
| H | 3.25820  | -0.29126 | -2.67826 | 3488.6892 | 3495.6879 | 3502.2455 |
| O | 2.48030  | -3.39928 | 0.33338  | 3516.9476 | 3521.8848 | 3530.0928 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | 1.50070  | -3.55729 | 0.39938  | 3532.1198 | 3541.243  | 3549.8267 |
|                                  | H | 2.91208  | -4.26000 | 0.28444  | 3554.1366 | 3563.4934 | 3567.1839 |
|                                  | O | 1.73355  | 0.54434  | 2.10935  | 3578.0134 | 3578.656  | 3595.1188 |
|                                  | H | 1.96547  | 1.06554  | 1.30234  | 3600.5432 | 3605.3067 | 3619.2846 |
|                                  | H | 0.95250  | -0.02472 | 1.92855  | 3624.6333 | 3632.9351 | 3633.3786 |
|                                  | O | 5.33043  | -2.79404 | -1.71814 | 3635.2881 | 3645.1334 | 3655.5424 |
|                                  | H | 6.02682  | -2.73991 | -2.38134 | 3682.6308 | 3708.7171 | 3709.7769 |
|                                  | H | 4.49452  | -2.60466 | -2.18245 | 3717.3849 | 3720.0837 | 3727.8262 |
|                                  | O | -0.26749 | -1.35711 | 2.18240  | 3737.08   | 3754.1881 | 3810.7737 |
|                                  | H | 0.14990  | -1.77022 | 2.96952  | 3859.5094 | 3868.6203 | 3870.037  |
|                                  | H | -1.18366 | -1.08043 | 2.42968  | 3870.2953 | 3874.6125 | 3875.8877 |
|                                  | O | -1.68932 | -0.78140 | -4.51183 | 3881.5276 | 3883.6363 | 3886.2975 |
|                                  | H | -2.67022 | -0.82861 | -4.31261 |           |           |           |
|                                  | H | -1.60474 | -0.67844 | -5.46542 |           |           |           |
| (H <sub>2</sub> O) <sub>35</sub> | O | 2.68164  | 3.38521  | 0.90752  | 26.6957   | 35.2218   | 39.4032   |
|                                  | H | 3.12521  | 3.43401  | 0.03702  | 41.907    | 44.5251   | 47.4548   |
|                                  | H | 2.35584  | 2.45009  | 0.96277  | 48.8021   | 50.4103   | 51.3939   |
|                                  | O | -2.82748 | 0.97738  | -2.95266 | 52.6      | 55.0454   | 55.863    |
|                                  | H | -3.70702 | 0.57324  | -2.87179 | 57.9471   | 58.8239   | 60.0402   |
|                                  | H | -2.25855 | 0.38140  | -2.39935 | 61.28     | 64.3381   | 65.0566   |
|                                  | O | 1.15879  | 2.82946  | -3.00242 | 68.3318   | 69.5168   | 70.6912   |
|                                  | H | 0.62332  | 3.55589  | -2.61784 | 71.5221   | 73.7053   | 74.8206   |
|                                  | H | 2.09008  | 3.03170  | -2.78163 | 75.7742   | 77.3929   | 78.6658   |
|                                  | O | -4.38436 | 0.54292  | 0.88748  | 79.3103   | 81.6597   | 81.9516   |
|                                  | H | -4.28374 | 1.50155  | 0.71158  | 83.0436   | 84.1424   | 85.2942   |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -4.67985 | 0.11852  | 0.04994  | 86.9833  | 88.485   | 89.983   |
| O | -1.88994 | 1.61075  | 4.07386  | 93.9046  | 95.8747  | 98.7997  |
| H | -1.99271 | 2.39423  | 3.50376  | 103.1382 | 104.5197 | 107.5676 |
| H | -2.70128 | 1.08392  | 3.96904  | 110.3605 | 113.2464 | 114.6322 |
| O | 2.74526  | -1.14131 | -2.99397 | 122.1318 | 122.8552 | 128.6345 |
| H | 2.22626  | -1.29123 | -3.80423 | 131.26   | 134.8739 | 137.9596 |
| H | 2.14765  | -0.59129 | -2.43675 | 142.7315 | 148.2515 | 150.9296 |
| O | 2.04703  | -1.48568 | 4.03157  | 157.5042 | 160.8406 | 161.8066 |
| H | 1.28493  | -0.96733 | 3.70575  | 165.2968 | 172.4246 | 173.2416 |
| H | 2.81797  | -0.90331 | 3.94462  | 175.0087 | 178.3263 | 181.4855 |
| O | -2.73193 | -3.45728 | 1.06569  | 184.6334 | 188.5139 | 191.3237 |
| H | -3.30379 | -3.53486 | 1.85366  | 194.9167 | 199.5204 | 202.1495 |
| H | -2.40756 | -2.52845 | 1.11641  | 203.9348 | 206.054  | 212.8033 |
| O | -1.11831 | -2.98005 | -2.96839 | 218.2671 | 223.6414 | 226.2606 |
| H | -0.64495 | -2.61068 | -3.73847 | 228.7056 | 233.4033 | 239.731  |
| H | -0.51411 | -3.64353 | -2.56050 | 242.2855 | 244.4186 | 257.9703 |
| O | 4.22007  | -0.54403 | 0.87474  | 260.117  | 264.2608 | 268.9064 |
| H | 4.18954  | -1.53006 | 0.85090  | 270.9968 | 273.5532 | 277.4715 |
| H | 4.54546  | -0.29692 | 1.76377  | 282.3931 | 288.3859 | 290.873  |
| O | 4.23879  | 3.05380  | 3.19052  | 302.6781 | 303.534  | 310.0278 |
| H | 3.79896  | 3.54565  | 3.89230  | 314.5963 | 316.0341 | 319.9337 |
| H | 3.74627  | 3.26764  | 2.36479  | 327.6274 | 335.2309 | 336.6652 |
| O | -0.51745 | 1.07407  | -4.77299 | 344.042  | 349.8378 | 357.5663 |
| H | 0.05764  | 1.70960  | -4.31279 | 359.715  | 363.149  | 365.8684 |
| H | -1.38236 | 1.10847  | -4.32553 | 370.7772 | 376.929  | 379.6051 |
| O | -4.30788 | -0.10873 | 3.53633  | 382.808  | 387.9599 | 396.9711 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -4.49128 | 0.10230  | 2.59100  | 400.7954 | 427.3674 | 447.2091 |
| H | -5.10926 | 0.11522  | 4.02300  | 461.0493 | 469.9628 | 472.6907 |
| O | -4.92613 | -0.66612 | -1.57818 | 474.8611 | 494.2894 | 496.6266 |
| H | -4.47275 | -1.55930 | -1.57438 | 497.3628 | 502.0553 | 511.8841 |
| H | -5.84360 | -0.84930 | -1.80969 | 519.1123 | 522.6985 | 527.9306 |
| O | 3.73220  | 3.08391  | -1.78130 | 535.6643 | 538.0079 | 542.6482 |
| H | 4.44327  | 3.64647  | -2.10808 | 549.9556 | 563.1937 | 569.9518 |
| H | 4.10900  | 2.15575  | -1.76421 | 575.0756 | 576.3185 | 580.8373 |
| O | 4.49534  | 0.33975  | 3.52018  | 584.3417 | 587.3163 | 597.2885 |
| H | 5.26388  | 0.19158  | 4.08191  | 599.8028 | 606.6325 | 617.9433 |
| H | 4.39047  | 1.32075  | 3.45377  | 624.2114 | 628.2423 | 633.6963 |
| O | -4.12204 | -3.01427 | 3.54136  | 639.5582 | 645.5213 | 652.7957 |
| H | -4.13501 | -2.03882 | 3.58794  | 662.8189 | 665.443  | 674.0037 |
| H | -3.54901 | -3.30110 | 4.26125  | 676.4446 | 679.0768 | 685.1013 |
| O | 0.48299  | -1.45069 | -4.86332 | 686.592  | 689.6826 | 705.6461 |
| H | 0.54433  | -1.68957 | -5.79491 | 709.4047 | 721.611  | 723.4383 |
| H | 0.11220  | -0.52923 | -4.84688 | 725.3479 | 728.8899 | 731.9275 |
| O | -3.75226 | -3.06515 | -1.55109 | 733.8032 | 736.2504 | 740.3255 |
| H | -2.97655 | -3.14813 | -2.13119 | 749.0737 | 764.8397 | 766.4451 |
| H | -3.45416 | -3.32162 | -0.65123 | 772.8647 | 777.0945 | 789.4658 |
| O | 4.71936  | 0.60699  | -1.71086 | 795.6214 | 806.6174 | 810.3012 |
| H | 4.66134  | 0.20810  | -0.81942 | 812.6409 | 825.749  | 837.0148 |
| H | 4.24421  | -0.00121 | -2.30529 | 841.6507 | 850.1671 | 860.0531 |
| O | 3.99745  | -3.27723 | 0.75169  | 866.6115 | 871.6119 | 885.7447 |
| H | 3.36542  | -3.57712 | -0.93941 | 891.5589 | 894.6049 | 906.7219 |
| H | 4.76884  | -3.81914 | 0.95020  | 914.1148 | 920.2283 | 941.4668 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 0.26008  | 4.82990  | 0.73605  | 948.8531  | 967.073   | 987.3806  |
| H | 1.10153  | 4.34151  | 0.86877  | 999.5456  | 1015.5387 | 1039.2697 |
| H | -0.19591 | 4.80945  | -0.83273 | 1063.8103 | 1068.2615 | 1082.1746 |
| O | 0.56764  | -4.73575 | -1.67916 | 1096.3035 | 1103.9827 | 1107.8069 |
| H | 0.10318  | -4.72394 | 0.20177  | 1154.5109 | 1195.9403 | 1214.012  |
| H | 0.61029  | -5.63975 | -2.00986 | 1647.9251 | 1649.1224 | 1657.9516 |
| O | -3.01187 | 3.51594  | -1.87103 | 1662.5421 | 1663.6321 | 1664.1194 |
| H | -2.91545 | 2.62818  | -2.28800 | 1667.7602 | 1668.9881 | 1669.8703 |
| H | -3.59894 | 3.40595  | -0.42378 | 1670.7298 | 1673.1835 | 1676.8895 |
| O | 2.97805  | -3.69983 | -1.83080 | 1677.8295 | 1685.6366 | 1686.3397 |
| H | 2.94287  | -2.80820 | -2.23755 | 1688.3738 | 1690.1975 | 1693.0589 |
| H | 1.50085  | -4.36530 | -1.73827 | 1695.6867 | 1698.2239 | 1699.0379 |
| O | -0.47150 | 4.74980  | -1.79624 | 1702.969  | 1707.4156 | 1709.81   |
| H | -2.13467 | 3.94780  | -1.89943 | 1712.0723 | 1715.6535 | 1721.534  |
| H | -0.45153 | 5.64701  | -2.14716 | 1724.3041 | 1729.112  | 1731.3022 |
| O | -0.10259 | -4.67363 | 1.15248  | 1732.467  | 1735.8428 | 1737.3364 |
| H | 1.31816  | -4.07506 | 2.10652  | 1743.3589 | 1747.6666 | 2792.7148 |
| H | -1.01458 | -4.33060 | 1.20329  | 2845.6681 | 3037.2769 | 3073.2651 |
| O | -3.98416 | 3.30575  | 0.51161  | 3121.4806 | 3124.4584 | 3172.9006 |
| H | -4.80374 | 3.81313  | 0.51845  | 3230.7532 | 3245.1037 | 3263.204  |
| H | -2.74391 | 3.77681  | 1.68859  | 3283.1961 | 3305.8665 | 3326.849  |
| O | 2.18802  | -3.83374 | 2.49710  | 3359.9368 | 3377.3388 | 3386.9573 |
| H | 3.28123  | -3.52829 | 1.43264  | 3395.3207 | 3405.5274 | 3409.9478 |
| H | 2.06636  | -3.04491 | 3.06875  | 3417.32   | 3431.7513 | 3438.7762 |
| O | -2.00765 | 3.93529  | 2.32688  | 3439.4903 | 3447.4107 | 3451.5827 |
| H | -2.25295 | 4.71850  | 2.83311  | 3456.3032 | 3457.7177 | 3471.7501 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.41204 | 4.43433  | 1.32118  | 3486.0077 | 3504.1238 | 3506.6432 |
|                                  | O | 0.00391  | 0.04145  | 2.80490  | 3513.7686 | 3517.177  | 3520.1759 |
|                                  | H | -0.54458 | 0.65201  | 3.34891  | 3546.8151 | 3559.6284 | 3566.4311 |
|                                  | H | -0.65079 | -0.37154 | 2.19606  | 3574.157  | 3589.8623 | 3590.1807 |
|                                  | O | 1.10677  | 0.51418  | -1.55176 | 3594.0437 | 3598.324  | 3599.6133 |
|                                  | H | 1.08202  | 1.38544  | -2.01106 | 3613.0643 | 3614.3962 | 3621.096  |
|                                  | H | 1.35527  | 0.66661  | -0.60604 | 3626.3128 | 3638.2003 | 3638.9837 |
|                                  | O | 1.85834  | 0.82655  | 1.00197  | 3653.3856 | 3672.9892 | 3676.9843 |
|                                  | H | 2.63866  | 0.22360  | 1.04512  | 3695.6315 | 3713.5931 | 3714.67   |
|                                  | H | 1.20589  | 0.57134  | 1.70302  | 3719.3146 | 3739.9653 | 3750.3007 |
|                                  | O | -1.91231 | -0.83928 | 1.03467  | 3857.1894 | 3860.3965 | 3861.9893 |
|                                  | H | -2.72293 | -0.29225 | 1.05996  | 3862.3888 | 3864.3931 | 3865.043  |
|                                  | H | -1.61791 | -0.79360 | 0.08821  | 3865.1395 | 3865.3872 | 3865.7284 |
|                                  | O | -1.24255 | -0.67624 | -1.54083 | 3869.7224 | 3870.7308 | 3872.3319 |
|                                  | H | -0.34251 | -0.25887 | -1.57744 |           |           |           |
|                                  | H | -1.17904 | -1.54570 | -2.00765 |           |           |           |
| (H <sub>2</sub> O) <sub>42</sub> | O | -1.89715 | -0.14018 | 3.89172  | 18.3812   | 24.9388   | 28.8987   |
|                                  | O | -2.06779 | 3.78901  | -1.53095 | 32.1265   | 34.9506   | 36.7749   |
|                                  | O | -2.82895 | -3.18666 | -2.13353 | 37.4387   | 39.1353   | 41.1909   |
|                                  | O | -2.54176 | 0.45276  | -3.79576 | 41.9964   | 44.5485   | 44.9112   |
|                                  | O | -2.68760 | -3.71956 | 2.03732  | 45.8659   | 46.4937   | 48.0906   |
|                                  | O | -1.86008 | 3.67203  | 2.36766  | 49.0592   | 50.6573   | 52.5695   |
|                                  | O | 1.94394  | 0.06712  | -3.83829 | 53.0712   | 53.9756   | 56.4163   |
|                                  | O | 2.64605  | 3.06778  | 2.07300  | 56.8792   | 57.2251   | 60.1145   |
|                                  | O | 2.07862  | -3.74080 | 1.60342  | 60.9657   | 62.2264   | 63.5221   |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | 2.56063  | -0.50534 | 3.94405  | 66.4308  | 67.4987  | 68.0946  |
| O | 1.97008  | -3.58926 | -2.39548 | 69.2789  | 70.3017  | 71.16    |
| O | 2.76031  | 3.83759  | -2.09673 | 72.0885  | 73.2703  | 73.9801  |
| O | -0.77143 | 5.50404  | 0.51940  | 74.1853  | 75.7337  | 79.1578  |
| O | -1.73472 | -2.10477 | -4.63534 | 80.9227  | 82.2692  | 83.4308  |
| O | -1.25194 | -2.92563 | 4.31648  | 86.1265  | 87.3308  | 87.8306  |
| O | -1.89042 | -5.13891 | -0.37721 | 89.8715  | 90.4003  | 92.3276  |
| O | -0.87117 | 2.29791  | 4.74158  | 103.6708 | 109.0199 | 109.9162 |
| O | -1.40444 | 3.10952  | -4.14790 | 112.0365 | 114.238  | 117.0387 |
| O | 1.87892  | 5.16569  | 0.38352  | 117.8981 | 118.6118 | 119.655  |
| O | 1.37133  | -3.14494 | 4.21090  | 121.756  | 124.0988 | 128.7082 |
| O | 0.90010  | -2.31759 | -4.78445 | 129.3336 | 133.3593 | 137.8678 |
| O | 0.75093  | -5.25163 | -0.49621 | 141.5586 | 144.8835 | 145.9256 |
| O | 1.22202  | 2.85936  | -4.23474 | 148.6724 | 153.6665 | 154.6585 |
| O | 1.76193  | 2.07897  | 4.67429  | 157.1212 | 159.9071 | 161.3429 |
| O | 5.00544  | -0.64270 | 2.44677  | 164.4741 | 167.4537 | 169.0244 |
| O | -4.58421 | 0.08004  | 2.91783  | 171.4297 | 175.772  | 178.8272 |
| O | 5.06048  | 2.15135  | -1.52020 | 179.9882 | 181.6782 | 182.3016 |
| O | -4.66920 | 2.84631  | -0.81135 | 184.521  | 186.2691 | 187.1846 |
| O | 4.64409  | -2.72072 | -1.79154 | 189.9292 | 190.5278 | 193.9298 |
| O | -5.31010 | -1.89260 | -1.37419 | 194.2493 | 195.7249 | 198.9281 |
| O | 4.64577  | -0.08810 | -2.91423 | 202.7769 | 207.3042 | 212.6405 |
| O | -5.08220 | 0.54199  | -2.46950 | 214.5409 | 217.062  | 219.6283 |
| O | 4.77001  | -2.99945 | 0.86312  | 220.8644 | 224.1789 | 224.9004 |
| O | -5.01667 | -2.10442 | 1.45394  | 226.4509 | 232.1962 | 239.8019 |
| O | 5.06453  | 1.75238  | 1.29049  | 242.7344 | 243.7173 | 245.8976 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | -4.53139 | 2.71983  | 1.84263  | 247.3667 | 251.4286 | 252.5435 |
| H | -1.46918 | -0.14436 | 3.02602  | 253.1227 | 257.1565 | 259.9666 |
| H | -1.56110 | 0.67914  | 4.32246  | 269.9845 | 282.2218 | 288.2489 |
| H | -1.86191 | 3.68244  | -2.48781 | 293.865  | 295.1121 | 297.7215 |
| H | -1.57566 | 3.07495  | -1.10621 | 300.3412 | 302.9722 | 305.1991 |
| H | -2.55276 | -3.98523 | -1.62997 | 305.8374 | 310.6558 | 312.0988 |
| H | -2.32884 | -2.47268 | -1.71782 | 313.6398 | 315.0943 | 317.1112 |
| H | -3.44910 | 0.54716  | -3.44671 | 319.2068 | 319.9306 | 321.5942 |
| H | -2.23348 | 1.34163  | -4.05008 | 322.4094 | 324.9701 | 325.581  |
| H | -3.49818 | -3.22656 | 1.80981  | 326.6606 | 329.0912 | 330.7401 |
| H | -2.44118 | -4.24752 | 1.25616  | 334.0586 | 335.4958 | 337.1274 |
| H | -2.79806 | 3.41546  | 2.27845  | 341.9196 | 343.3231 | 344.877  |
| H | -1.54624 | 3.31506  | 3.21840  | 347.116  | 351.2495 | 352.6889 |
| H | 1.60433  | -0.73094 | -4.30514 | 353.5987 | 359.939  | 360.0455 |
| H | 1.49499  | 0.04955  | -2.98377 | 364.3902 | 365.9434 | 367.9566 |
| H | 2.04510  | 2.40847  | 1.70319  | 369.0055 | 377.2469 | 378.2646 |
| H | 2.42663  | 3.89173  | 1.58216  | 387.1549 | 394.277  | 408.2699 |
| H | 1.84779  | -3.67832 | 2.55875  | 418.4976 | 419.29   | 424.2602 |
| H | 1.71205  | -2.93350 | 1.22087  | 430.8668 | 435.4782 | 436.8655 |
| H | 3.42273  | -0.62406 | 3.50130  | 441.4529 | 442.4309 | 446.353  |
| H | 2.20002  | -1.39168 | 4.12922  | 453.1291 | 456.5295 | 459.2892 |
| H | 1.67266  | -3.27037 | -3.26620 | 460.9268 | 472.9543 | 473.5967 |
| H | 2.90868  | -3.34141 | -2.29252 | 486.3796 | 486.4832 | 492.3178 |
| H | 3.57839  | 3.35283  | -1.88003 | 495.0944 | 503.0222 | 519.1556 |
| H | 2.47916  | 4.31012  | -1.29325 | 527.3192 | 534.217  | 534.8577 |
| H | -1.15869 | 4.98161  | 1.25283  | 538.0829 | 543.6277 | 545.6708 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | -1.22344 | 5.17957  | -0.27866 | 556.0302  | 569.4755  | 571.8168  |
| H | -2.03002 | -1.18823 | -4.44674 | 573.9262  | 577.6547  | 578.809   |
| H | -2.13659 | -2.65339 | -3.93857 | 582.8327  | 587.2872  | 589.6095  |
| H | -1.74605 | -3.28868 | 3.55047  | 592.1223  | 595.4252  | 597.9746  |
| H | -1.50526 | -1.98604 | 4.36576  | 612.4973  | 617.119   | 618.6237  |
| H | -0.88945 | -5.18375 | -0.42768 | 623.1369  | 632.6935  | 636.9443  |
| H | -2.19843 | -6.05104 | -0.42146 | 653.909   | 656.0106  | 667.5571  |
| H | 0.13037  | 2.22557  | 4.73151  | 670.524   | 673.5464  | 675.5386  |
| H | -1.10405 | 2.65510  | 5.60586  | 678.0571  | 679.3113  | 686.1438  |
| H | -1.65189 | 3.66853  | -4.89277 | 692.6488  | 693.6679  | 701.7486  |
| H | -0.40377 | 3.02739  | -4.18427 | 709.3436  | 713.4541  | 717.0901  |
| H | 2.26688  | 6.04272  | 0.48055  | 719.9063  | 721.9375  | 722.5537  |
| H | 0.88806  | 5.30028  | 0.42695  | 727.0346  | 730.1995  | 731.2044  |
| H | 0.36907  | -3.07974 | 4.25690  | 732.107   | 736.7848  | 737.7694  |
| H | 1.63874  | -3.69519 | 4.95533  | 767.9049  | 770.7528  | 772.209   |
| H | 1.10148  | -2.65051 | -5.66594 | 776.3957  | 780.3429  | 781.7659  |
| H | -0.10015 | -2.25416 | -4.73219 | 784.2836  | 788.3475  | 791.6849  |
| H | 1.16702  | -4.75477 | -1.23214 | 792.9949  | 793.6745  | 805.7319  |
| H | 1.19240  | -4.92959 | 0.31032  | 823.1233  | 824.9323  | 829.1556  |
| H | 1.74093  | 3.25942  | -3.50396 | 834.65    | 850.6579  | 854.7858  |
| H | 1.49960  | 1.92675  | -4.27736 | 1029.2056 | 1030.1126 | 1034.6432 |
| H | 2.14128  | 2.59165  | 3.93879  | 1039.3494 | 1055.1346 | 1070.1373 |
| H | 2.05985  | 1.15538  | 4.52832  | 1080.8523 | 1082.7133 | 1084.9307 |
| H | 5.03916  | 0.23648  | 1.97138  | 1090.9364 | 1094.3941 | 1103.628  |
| H | 5.79512  | -0.66814 | 2.99916  | 1663.2195 | 1663.9482 | 1665.7195 |
| H | -3.71249 | 0.02120  | 3.35458  | 1667.88   | 1668.4561 | 1669.7507 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | -4.61597 | 0.96891  | 2.51064  | 1670.1924 | 1671.4544 | 1672.9179 |
| H | 4.91775  | 1.29820  | -2.02019 | 1673.6017 | 1674.683  | 1675.4688 |
| H | 5.88952  | 2.51318  | -1.85326 | 1679.8339 | 1681.7338 | 1683.4525 |
| H | -3.83298 | 3.22578  | -1.14647 | 1684.3895 | 1685.7741 | 1688.3389 |
| H | -4.82883 | 2.03083  | -1.32593 | 1698.08   | 1698.3775 | 1700.1403 |
| H | 4.70927  | -2.80164 | -0.79751 | 1700.3839 | 1701.3493 | 1702.4309 |
| H | 5.35639  | -3.26562 | -2.14475 | 1711.0725 | 1713.2501 | 1713.6598 |
| H | -4.58046 | -2.45925 | -1.68894 | 1714.8863 | 1722.3056 | 1726.1071 |
| H | -5.25756 | -1.92240 | -0.39740 | 1726.6177 | 1727.3615 | 1728.9126 |
| H | 3.76118  | -0.05957 | -3.32797 | 1729.909  | 1731.4725 | 1732.8213 |
| H | 4.70290  | -0.95885 | -2.47365 | 3045.3823 | 3061.2316 | 3073.9168 |
| H | -5.17594 | -0.35230 | -2.03382 | 3080.6596 | 3100.4543 | 3128.6127 |
| H | -5.87315 | 0.65173  | -3.00934 | 3129.4084 | 3139.8317 | 3172.9164 |
| H | 4.90106  | -2.17260 | 1.36943  | 3174.3984 | 3182.7636 | 3183.3054 |
| H | 3.92832  | -3.37264 | 1.18794  | 3447.2773 | 3451.526  | 3451.733  |
| H | -5.79534 | -2.51483 | 1.84756  | 3458.1095 | 3472.5535 | 3478.4629 |
| H | -4.87238 | -1.25919 | 1.96735  | 3511.0984 | 3513.9477 | 3515.5891 |
| H | 5.10154  | 1.84636  | 0.31693  | 3519.2355 | 3526.5949 | 3536.261  |
| H | 4.30843  | 2.29702  | 1.58319  | 3551.085  | 3558.0861 | 3560.5095 |
| H | -5.25504 | 3.26711  | 2.16806  | 3561.721  | 3563.4411 | 3568.6411 |
| H | -4.60630 | 2.73640  | 0.84555  | 3581.881  | 3587.7108 | 3589.6138 |
| H | -1.96799 | 0.78436  | 0.90001  | 3590.4979 | 3597.1946 | 3601.5038 |
| H | -1.87880 | 1.41220  | 1.28745  | 3617.9412 | 3618.5166 | 3620.378  |
| H | 0.77940  | 0.51506  | 1.58909  | 3622.0924 | 3627.6615 | 3633.8584 |
| H | -0.53113 | -1.54740 | 1.06626  | 3663.6321 | 3665.6659 | 3667.0909 |
| H | 1.19914  | 0.26478  | 2.15359  | 3670.5279 | 3671.1326 | 3672.3283 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | -0.99283 | -2.06858 | 1.33276  | 3673.8886 | 3679.817  | 3683.7263 |
|                                  | H | -0.19212 | 1.15280  | -1.69661 | 3683.9341 | 3689.6001 | 3700.8932 |
|                                  | H | 0.38257  | 2.57690  | 0.08303  | 3834.4057 | 3835.2191 | 3836.2605 |
|                                  | H | -0.72323 | 0.94241  | -2.17342 | 3837.3327 | 3838.5204 | 3841.9186 |
|                                  | H | 2.22317  | 0.92718  | -0.73532 | 3858.032  | 3859.8421 | 3861.286  |
|                                  | H | 2.23475  | 1.58826  | -1.07562 | 3861.4494 | 3861.5972 | 3861.8654 |
|                                  | H | -0.07677 | 2.78313  | 0.62960  | 3862.0869 | 3862.739  | 3863.0886 |
|                                  | H | -2.53062 | -0.30501 | -1.26027 | 3864.1686 | 3864.7559 | 3865.4727 |
|                                  | H | 0.15196  | -2.02826 | -1.73351 | 4383.0916 | 4404.9915 | 4427.3294 |
|                                  | H | -2.76499 | -0.62180 | -0.63064 | 4435.3096 | 4436.5066 | 4441.1376 |
|                                  | H | 2.40849  | -1.18866 | 0.06796  | 4445.8022 | 4446.9242 | 4450.6862 |
|                                  | H | -0.27476 | -1.43220 | -1.60803 |           |           |           |
|                                  | H | 2.15312  | -1.60527 | -0.49194 |           |           |           |
| (H <sub>2</sub> O) <sub>54</sub> | O | -6.36191 | -1.25445 | 1.60858  | 34.4604   | 34.9601   | 36.1505   |
|                                  | H | -6.44129 | -0.28680 | 1.54221  | 37.0705   | 37.5626   | 38.5789   |
|                                  | H | -5.84051 | -1.52309 | 0.82658  | 39.5891   | 40.8623   | 41.9164   |
|                                  | O | -4.76467 | -2.03058 | -0.60235 | 42.863    | 45.4969   | 47.1264   |
|                                  | H | -3.98211 | -1.44459 | -0.64526 | 48.1477   | 48.8567   | 49.8388   |
|                                  | H | -5.32929 | -1.78291 | -1.38337 | 50.8017   | 53.0122   | 53.9101   |
|                                  | O | -4.88920 | -2.38566 | 3.63737  | 56.2224   | 56.4816   | 57.8454   |
|                                  | H | -5.46364 | -1.97885 | 2.94788  | 59.0228   | 60.2235   | 60.4033   |
|                                  | H | -4.48654 | -3.18977 | 3.23443  | 61.2011   | 62.641    | 63.2732   |
|                                  | O | -6.24915 | -1.22309 | -2.68188 | 64.1151   | 65.2385   | 66.2752   |
|                                  | H | -6.38268 | -0.27946 | -2.44231 | 66.9189   | 68.5439   | 68.6219   |
|                                  | H | -5.63632 | -1.25597 | -3.43400 | 69.0585   | 70.6169   | 70.7965   |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | -6.64524 | 1.61423  | 1.15870  | 71.0103  | 72.3522  | 73.2499  |
| H | -7.51220 | 1.86804  | 1.49417  | 73.9774  | 75.095   | 76.1304  |
| H | -5.98816 | 2.16028  | 1.66444  | 76.8469  | 78.197   | 80.319   |
| O | -4.03781 | -4.59927 | -0.43050 | 81.025   | 81.8409  | 83.2374  |
| H | -4.35684 | -3.65945 | -0.52725 | 84.6889  | 85.7333  | 86.8368  |
| H | -4.72747 | -5.16155 | -0.79988 | 88.3897  | 89.5378  | 91.0843  |
| O | -6.52390 | 1.41116  | -1.71787 | 91.8591  | 92.6293  | 94.7944  |
| H | -5.77099 | 1.97950  | -1.94650 | 95.381   | 97.802   | 98.131   |
| H | -6.59605 | 1.45815  | -0.74459 | 99.2173  | 101.024  | 104.4877 |
| O | -3.63058 | -4.57778 | 2.47145  | 105.2509 | 106.1502 | 109.2165 |
| H | -2.66756 | -4.41052 | 2.45839  | 111.3936 | 118.0376 | 119.0144 |
| H | -3.86608 | -4.68636 | 1.53463  | 123.49   | 128.6375 | 130.2288 |
| O | -3.12192 | -0.75368 | 4.50935  | 133.3372 | 136.5995 | 138.5998 |
| H | -3.42912 | -0.52771 | 5.39476  | 141.3812 | 142.7806 | 144.3299 |
| H | -3.83313 | -1.39041 | 4.13478  | 146.9255 | 147.3511 | 149.9584 |
| O | -3.96741 | -1.53067 | -4.57709 | 151.1053 | 152.6151 | 154.562  |
| H | -3.55067 | -0.69801 | -4.25151 | 156.5011 | 158.9097 | 160.2286 |
| H | -4.15292 | -1.40539 | -5.51426 | 160.7226 | 163.1651 | 164.4818 |
| O | -4.87030 | 3.03564  | 2.62861  | 167.5342 | 169.5459 | 172.1285 |
| H | -4.47638 | 3.86844  | 2.31642  | 173.2749 | 175.6697 | 178.4029 |
| H | -4.10352 | 2.49149  | 2.90669  | 180.1479 | 182.2333 | 183.6735 |
| O | -1.55564 | -4.39926 | -1.63770 | 186.2602 | 187.1273 | 188.1308 |
| H | -2.40514 | -4.61916 | -1.19315 | 192.4521 | 193.7948 | 196.4058 |
| H | -0.92273 | -5.13503 | -1.49631 | 198.7897 | 202.6195 | 204.8471 |
| O | -0.88745 | -3.82580 | 2.27964  | 206.4167 | 206.8267 | 211.0032 |
| H | -0.20024 | -4.51009 | 2.09278  | 214.6424 | 217.0415 | 219.3001 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -0.83692 | -3.20430 | 1.52767  | 222.2627 | 223.4234 | 224.7786 |
| O | -4.22092 | 2.91825  | -2.74161 | 228.9333 | 232.0546 | 234.3034 |
| H | -3.71789 | 2.10884  | -3.01906 | 237.734  | 238.5376 | 239.2725 |
| H | -4.61254 | 3.29297  | -3.53814 | 246.0024 | 247.619  | 254.2479 |
| O | -2.53155 | 1.56345  | 3.14451  | 259.6559 | 261.3194 | 263.1805 |
| H | -1.87424 | 1.99171  | 3.73486  | 265.3768 | 266.6971 | 268.549  |
| H | -2.74567 | 0.69292  | 3.56029  | 271.0414 | 275.3055 | 280.5681 |
| O | -1.80712 | -3.51438 | -4.25088 | 286.8339 | 289.0635 | 291.9526 |
| H | -1.81467 | -3.85633 | -3.32922 | 294.9327 | 295.2608 | 297.023  |
| H | -2.53738 | -2.87486 | -4.32953 | 302.7634 | 304.2484 | 308.1861 |
| O | -2.83618 | 0.65711  | -3.36894 | 310.4457 | 315.9148 | 319.5453 |
| H | -1.99523 | 0.90536  | -3.80518 | 322.1428 | 325.0341 | 325.7568 |
| H | -2.60565 | 0.23291  | -2.49396 | 332.1635 | 332.4789 | 334.8259 |
| O | -0.90572 | -2.47458 | 4.68852  | 338.078  | 338.8845 | 341.7439 |
| H | -0.89924 | -2.99121 | 3.85107  | 343.6347 | 344.6961 | 345.6275 |
| H | -1.68149 | -1.87770 | 4.64167  | 348.9485 | 350.2486 | 355.2594 |
| O | 0.65135  | -6.04588 | -1.26318 | 356.0551 | 356.9503 | 358.9212 |
| H | 0.70592  | -6.97603 | -1.50808 | 364.429  | 366.3203 | 366.6222 |
| H | 1.28043  | -5.55725 | -1.86772 | 377.182  | 379.6465 | 382.6685 |
| O | -3.27149 | 5.27563  | 1.67432  | 394.8269 | 409.1699 | 416.6749 |
| H | -3.59850 | 6.18065  | 1.72228  | 417.5273 | 430.5011 | 432.0916 |
| H | -3.17017 | 5.05772  | 0.72002  | 457.143  | 458.0314 | 465.8102 |
| O | 1.05769  | -5.63950 | 1.57841  | 472.5139 | 472.9024 | 476.2812 |
| H | 1.95972  | -5.32477 | 1.77178  | 476.9513 | 479.2253 | 484.6639 |
| H | 1.01129  | -5.79445 | 0.61728  | 495.071  | 499.1435 | 503.6951 |
| O | -2.73080 | 4.31171  | -0.82161 | 513.908  | 516.1902 | 519.7851 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -3.30671 | 3.93826  | -1.52113 | 529.9527 | 546.7182 | 550.9018 |
| H | -2.00019 | 4.77704  | -1.27309 | 552.612  | 555.1679 | 556.3002 |
| O | 0.74387  | -3.08467 | -4.80575 | 562.9993 | 567.7845 | 570.3876 |
| H | 0.90112  | -3.56576 | -5.62656 | 575.2062 | 576.9065 | 580.8209 |
| H | -0.23412 | -3.19193 | -4.61632 | 591.2422 | 591.6078 | 593.4623 |
| O | -0.63097 | 2.89345  | 4.69661  | 597.0302 | 597.6384 | 600.4111 |
| H | 0.21029  | 2.36179  | 4.83593  | 607.7488 | 610.435  | 611.0582 |
| H | -0.90982 | 3.17197  | 5.57597  | 612.7973 | 613.9168 | 620.166  |
| O | -0.55792 | 1.53276  | -4.72437 | 626.3941 | 627.3825 | 627.6157 |
| H | -0.77898 | 1.98056  | -5.54853 | 631.3514 | 635.0097 | 648.2007 |
| H | -0.15545 | 2.21695  | -4.12774 | 653.3691 | 658.9338 | 667.1884 |
| O | 1.37894  | -1.32382 | 4.95829  | 669.3318 | 670.9665 | 674.0456 |
| H | 1.77263  | -1.70546 | 5.75106  | 675.6723 | 677.735  | 682.1348 |
| H | 0.45952  | -1.74663 | 4.87124  | 683.177  | 687.4427 | 691.0228 |
| O | 2.25366  | -4.67430 | -2.88289 | 693.9009 | 697.8825 | 700.3124 |
| H | 2.90891  | -4.11978 | -2.40777 | 704.6525 | 708.716  | 711.1094 |
| H | 1.75897  | -4.08264 | -3.47963 | 717.5611 | 718.2602 | 720.54   |
| O | -0.56318 | 5.05524  | 2.87002  | 723.1742 | 724.4869 | 727.7997 |
| H | -1.46046 | 5.11186  | 2.49816  | 731.0819 | 733.6529 | 737.9014 |
| H | -0.58173 | 4.33686  | 3.53400  | 740.6782 | 743.8124 | 747.9359 |
| O | 1.52822  | -0.42507 | -5.08694 | 749.5919 | 752.1991 | 754.3362 |
| H | 1.23652  | -1.35652 | -4.97324 | 758.1587 | 759.9617 | 762.0566 |
| H | 0.73541  | 0.13323  | -5.00358 | 774.877  | 776.6067 | 783.7151 |
| O | 1.51940  | 1.46508  | 5.19062  | 788.5778 | 797.5285 | 799.2264 |
| H | 1.41984  | 0.49424  | 5.09699  | 800.6288 | 802.2905 | 808.6738 |
| H | 2.39972  | 1.68251  | 4.82321  | 817.6868 | 819.6204 | 827.4518 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 3.62360  | -4.55222 | 2.38390  | 828.5888  | 831.529   | 837.7534  |
| H | 3.87935  | -4.98924 | 3.20389  | 841.3027  | 843.7168  | 851.0302  |
| H | 3.34457  | -3.62844 | 2.62870  | 851.5413  | 860.9261  | 868.4322  |
| O | -0.56892 | 5.66114  | -2.23347 | 876.1929  | 878.4049  | 883.8894  |
| H | -0.86454 | 6.28688  | -2.90417 | 889.9961  | 892.8956  | 906.0074  |
| H | -0.16945 | 4.89290  | -2.70651 | 909.0772  | 916.014   | 926.3991  |
| O | 2.91818  | -1.99406 | 2.75145  | 932.4793  | 936.1457  | 941.3118  |
| H | 3.73235  | -1.46564 | 2.97696  | 945.1607  | 951.7918  | 955.3199  |
| H | 2.29235  | -1.79962 | 3.48595  | 957.0404  | 964.1735  | 966.3302  |
| O | 0.58031  | 3.34237  | -3.06891 | 969.2856  | 979.2446  | 982.2081  |
| H | 1.50878  | 3.37650  | -3.38152 | 1000.6775 | 1009.2144 | 1014.6295 |
| H | 0.59773  | 3.02303  | -2.12194 | 1033.5013 | 1038.4522 | 1040.5408 |
| O | 3.99573  | -3.01142 | -1.44321 | 1047.2661 | 1063.9168 | 1073.6884 |
| H | 4.63534  | -3.37177 | -0.77085 | 1079.9414 | 1083.6369 | 1086.3043 |
| H | 4.51154  | -2.38421 | -1.98473 | 1099.8513 | 1108.3322 | 1111.6543 |
| O | 1.48534  | 4.50190  | 1.17632  | 1170.0614 | 1172.7768 | 1227.5977 |
| H | 0.75039  | 4.75783  | 1.79048  | 1640.6136 | 1642.8456 | 1653.0032 |
| H | 1.66687  | 5.27199  | 0.59213  | 1657.788  | 1659.2311 | 1660.6251 |
| O | 5.65757  | -3.80614 | 0.52019  | 1661.9058 | 1663.6848 | 1664.6263 |
| H | 6.07738  | -2.99435 | 0.86396  | 1665.8701 | 1667.2312 | 1668.1105 |
| H | 5.06233  | -4.13248 | 1.22336  | 1668.8921 | 1670.5147 | 1671.5574 |
| O | 2.00664  | 6.31828  | -0.84317 | 1672.9853 | 1673.2298 | 1674.1319 |
| H | 2.70934  | 5.82774  | -1.30435 | 1675.3366 | 1678.4399 | 1679.3133 |
| H | 1.19527  | 6.21252  | -1.36732 | 1679.9867 | 1681.3922 | 1682.3214 |
| O | 3.35434  | 0.63089  | -3.46556 | 1682.4812 | 1688.1094 | 1691.3839 |
| H | 3.00396  | 0.63959  | -2.53416 | 1696.4264 | 1699.0225 | 1699.4771 |

|   |         |          |          |           |           |           |
|---|---------|----------|----------|-----------|-----------|-----------|
| H | 2.67383 | 0.16947  | -4.03212 | 1702.7133 | 1703.055  | 1704.0128 |
| O | 4.12846 | 1.96919  | 4.18946  | 1704.3691 | 1705.2098 | 1706.6715 |
| H | 4.07192 | 2.63274  | 3.43973  | 1708.7952 | 1710.2499 | 1712.2913 |
| H | 4.66342 | 2.38605  | 4.87423  | 1713.852  | 1716.9612 | 1718.3516 |
| O | 5.09493 | -0.61586 | 3.46435  | 1720.4473 | 1722.9232 | 1727.5042 |
| H | 4.87573 | 0.32231  | 3.62771  | 1727.9217 | 1731.6623 | 1732.5618 |
| H | 5.76719 | -0.66658 | 2.75851  | 1733.9348 | 1737.1734 | 1739.8091 |
| O | 3.23105 | 3.19881  | -4.04739 | 1745.1651 | 1750.0932 | 1755.8088 |
| H | 3.35753 | 2.21253  | -3.89047 | 2696.5737 | 2856.1692 | 2993.7853 |
| H | 3.40165 | 3.35791  | -4.98223 | 3051.692  | 3089.6372 | 3103.6797 |
| O | 5.45711 | -1.00841 | -2.90916 | 3104.5629 | 3129.388  | 3148.0651 |
| H | 4.74658 | -0.40618 | -3.24159 | 3164.8133 | 3165.9818 | 3168.6342 |
| H | 5.97123 | -1.29004 | -3.67378 | 3186.5676 | 3190.3144 | 3204.2915 |
| O | 4.00889 | 3.66842  | 2.18182  | 3223.6226 | 3254.7647 | 3261.2449 |
| H | 4.35079 | 3.21666  | 1.38456  | 3270.8874 | 3277.4723 | 3282.0327 |
| H | 3.11541 | 3.98591  | 1.93611  | 3287.8922 | 3297.2444 | 3319.6072 |
| O | 6.85837 | -1.28858 | 1.34840  | 3333.6922 | 3369.3514 | 3371.4505 |
| H | 6.83939 | -0.66040 | 0.57397  | 3388.7355 | 3391.8783 | 3396.2488 |
| H | 7.78586 | -1.37974 | 1.59353  | 3409.0607 | 3415.0441 | 3416.31   |
| O | 4.23122 | 4.68631  | -1.95346 | 3418.3986 | 3421.8373 | 3432.9798 |
| H | 4.00912 | 4.23508  | -2.79689 | 3436.2973 | 3442.522  | 3446.0825 |
| H | 5.01421 | 5.22417  | -2.11890 | 3463.0912 | 3463.6411 | 3469.7424 |
| O | 6.76951 | 0.38944  | -0.73514 | 3479.9699 | 3482.4486 | 3484.0921 |
| H | 6.38749 | -0.06872 | -1.50620 | 3487.0956 | 3490.8524 | 3492.5934 |
| H | 6.17902 | 1.15023  | -0.55949 | 3507.5643 | 3517.6658 | 3526.7211 |
| O | 4.80504 | 2.38345  | -0.22569 | 3531.306  | 3536.6334 | 3543.5062 |

|                                  |   |          |          |          |           |           |           |
|----------------------------------|---|----------|----------|----------|-----------|-----------|-----------|
|                                  | H | 4.02901  | 1.80050  | -0.39802 | 3544.5264 | 3551.619  | 3552.9746 |
|                                  | H | 4.69853  | 3.14834  | -0.82051 | 3556.111  | 3557.4538 | 3559.2412 |
|                                  | O | -2.42784 | -0.39386 | -0.94449 | 3561.6204 | 3570.6355 | 3571.8709 |
|                                  | H | -2.30338 | 0.38974  | -0.36323 | 3572.9189 | 3584.1281 | 3589.3522 |
|                                  | H | -1.70585 | -1.02474 | -0.69871 | 3596.2378 | 3599.3267 | 3602.5012 |
|                                  | O | -0.60938 | -2.26240 | -0.14066 | 3607.7322 | 3614.328  | 3616.202  |
|                                  | H | 0.35881  | -2.10251 | -0.15755 | 3627.0552 | 3630.9882 | 3645.0871 |
|                                  | H | -0.81226 | -3.03001 | -0.72180 | 3647.2443 | 3656.8079 | 3657.1699 |
|                                  | O | -1.85097 | 1.87556  | 0.51216  | 3658.6038 | 3661.3187 | 3669.1642 |
|                                  | H | -2.06657 | 1.75192  | 1.47119  | 3674.44   | 3677.5932 | 3683.6456 |
|                                  | H | -2.28300 | 2.69444  | 0.20652  | 3684.0968 | 3703.3655 | 3707.8661 |
|                                  | O | 2.13967  | -1.65072 | 0.10389  | 3725.3244 | 3733.3774 | 3741.6617 |
|                                  | H | 2.38305  | -1.75262 | 1.05479  | 3855.7485 | 3855.9731 | 3858.8257 |
|                                  | H | 2.78473  | -2.18744 | -0.41502 | 3862.4272 | 3862.5687 | 3863.7138 |
|                                  | O | 0.61500  | 2.58042  | -0.48844 | 3864.5803 | 3864.8899 | 3865.2657 |
|                                  | H | -0.22367 | 2.24473  | -0.09338 | 3865.6811 | 3866.199  | 3867.1457 |
|                                  | H | 0.93715  | 3.28909  | 0.13677  | 3867.6934 | 3868.1112 | 3868.2241 |
|                                  | O | 2.62778  | 0.80740  | -0.88211 | 3869.5464 | 3870.0339 | 3871.4396 |
|                                  | H | 2.46180  | -0.07304 | -0.45300 |           |           |           |
|                                  | H | 1.84611  | 1.37417  | -0.67944 |           |           |           |
| (H <sub>2</sub> O) <sub>80</sub> | O | -2.94115 | 6.40224  | -1.11815 | 35.9325   | 37.0234   | 37.8437   |
|                                  | H | -3.24285 | 7.26928  | -1.41172 | 37.9559   | 38.4385   | 38.9444   |
|                                  | H | -3.12386 | 5.77653  | -1.86927 | 39.4497   | 39.6254   | 39.9096   |
|                                  | O | -3.86130 | 5.20505  | 1.25741  | 40.5896   | 43.0256   | 43.3785   |
|                                  | H | -3.61930 | 5.74023  | 0.47134  | 45.5731   | 47.9394   | 48.9712   |

|   |          |         |          |          |          |          |
|---|----------|---------|----------|----------|----------|----------|
| H | -3.35950 | 5.56323 | 2.02441  | 50.1156  | 50.2688  | 50.9012  |
| O | -3.28515 | 4.55329 | -3.07696 | 51.2144  | 51.9001  | 52.1014  |
| H | -4.16841 | 4.21199 | -3.31716 | 52.5594  | 53.9275  | 54.1632  |
| H | -2.84539 | 3.78643 | -2.62891 | 54.7844  | 55.3916  | 55.8615  |
| O | -6.10199 | 3.49641 | 1.20601  | 56.1103  | 56.8057  | 57.175   |
| H | -5.32602 | 4.09853 | 1.25606  | 57.7588  | 58.9472  | 59.1237  |
| H | -6.86674 | 4.05286 | 1.39510  | 61.0433  | 61.6714  | 62.3457  |
| O | -6.40426 | 1.22363 | 3.10185  | 63.2233  | 64.0986  | 64.5676  |
| H | -6.24466 | 1.97880 | 2.50802  | 64.6934  | 66.48    | 66.9656  |
| H | -5.72454 | 1.29943 | 3.80360  | 67.7035  | 67.768   | 68.855   |
| O | -2.17148 | 5.86037 | 3.37569  | 69.5321  | 69.9826  | 70.7251  |
| H | -2.30270 | 6.64188 | 3.92459  | 71.527   | 72.3421  | 72.5053  |
| H | -1.25184 | 5.93994 | 2.99588  | 72.7263  | 73.1528  | 74.0504  |
| O | -2.31839 | 3.70067 | 5.46120  | 74.7515  | 74.8906  | 76.0401  |
| H | -2.28373 | 4.33048 | 4.72205  | 76.5539  | 77.4407  | 77.8615  |
| H | -2.98433 | 3.02564 | 5.23510  | 78.5293  | 79.4086  | 79.8341  |
| O | -4.10024 | 1.43898 | 4.76342  | 80.8916  | 81.0501  | 81.643   |
| H | -3.86430 | 0.72884 | 5.38891  | 82.3696  | 82.8091  | 82.8618  |
| H | -3.61965 | 1.22272 | 3.93023  | 83.5885  | 85.4063  | 87.0089  |
| O | 1.20688  | 4.62054 | -4.28255 | 88.5641  | 88.7644  | 89.3999  |
| H | 2.03250  | 4.23396 | -4.65684 | 90.2278  | 90.3615  | 90.8817  |
| H | 1.47530  | 5.35573 | -3.69302 | 91.4084  | 92.3795  | 93.0774  |
| O | 1.93647  | 6.55158 | -2.32662 | 93.94    | 95.8077  | 95.9338  |
| H | 2.07052  | 7.45258 | -2.64253 | 96.4155  | 97.3301  | 98.2501  |
| H | 1.21821  | 6.62291 | -1.64248 | 99.9933  | 101.0345 | 101.7877 |
| O | -1.46792 | 4.29239 | -5.42021 | 103.1749 | 103.6044 | 104.1338 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -2.06353 | 4.49768  | -4.67832 | 105.3874 | 106.0824 | 107.3798 |
| H | -0.56708 | 4.49879  | -5.11167 | 107.4994 | 109.3775 | 110.7411 |
| O | -0.03967 | 6.90549  | -0.51028 | 112.4114 | 114.0656 | 115.2815 |
| H | 0.10418  | 6.63183  | 0.42081  | 117.785  | 119.1261 | 119.5776 |
| H | -0.95246 | 6.65634  | -0.73265 | 122.1881 | 124.0049 | 125.6837 |
| O | 0.22990  | 5.91390  | 2.14322  | 126.906  | 128.8352 | 130.2764 |
| H | 0.29209  | 4.96035  | 1.88874  | 130.8579 | 132.4307 | 135.2887 |
| H | 1.08491  | 6.03967  | 2.62789  | 135.8664 | 137.0555 | 138.0193 |
| O | 4.60498  | 5.72130  | -1.37492 | 140.867  | 142.215  | 143.9256 |
| H | 3.70149  | 5.96876  | -1.64690 | 145.6217 | 146.3104 | 147.4449 |
| H | 4.83989  | 4.95196  | -1.92134 | 149.0745 | 150.6484 | 151.9545 |
| O | 4.15480  | 4.45370  | 1.07125  | 153.9054 | 155.3812 | 157.129  |
| H | 3.46660  | 3.93711  | 0.60099  | 158.4604 | 159.7825 | 161.0474 |
| H | 4.47835  | 5.04086  | 0.35183  | 162.4042 | 163.3589 | 164.749  |
| O | 2.68578  | 5.69382  | 3.31387  | 165.8364 | 166.5618 | 170.6309 |
| H | 2.59592  | 4.95062  | 3.94264  | 171.0268 | 173.4987 | 175.0936 |
| H | 3.23847  | 5.35290  | 2.58482  | 176.5696 | 176.8399 | 177.6761 |
| O | 0.41588  | 0.12147  | -6.17919 | 179.5582 | 180.2875 | 181.8481 |
| H | 0.19696  | -0.82267 | -6.39001 | 182.8868 | 184.8607 | 185.8681 |
| H | -0.40250 | 0.67373  | -6.30139 | 186.6291 | 186.9256 | 189.7803 |
| O | 3.04455  | 0.61642  | -6.26730 | 190.8165 | 192.3617 | 193.3904 |
| H | 3.34531  | 0.71406  | -7.17828 | 196.8214 | 197.6683 | 198.9401 |
| H | 2.05766  | 0.48974  | -6.32292 | 200.72   | 201.3881 | 202.4303 |
| O | -1.82324 | 1.63479  | -6.23427 | 206.3301 | 206.6892 | 208.6698 |
| H | -1.69230 | 2.57428  | -5.97248 | 210.8094 | 214.3336 | 214.5297 |
| H | -2.57082 | 1.31133  | -5.70308 | 216.1184 | 219.8193 | 222.3634 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | 3.50757  | 3.32064  | -5.14841 | 223.6069 | 226.9457 | 230.0882 |
| H | 3.35051  | 2.41021  | -5.45520 | 231.562  | 232.2935 | 235.8967 |
| H | 4.16274  | 3.26380  | -4.42970 | 237.6313 | 241.0437 | 243.8653 |
| O | 5.53673  | 3.43948  | -3.05152 | 245.5897 | 246.9651 | 249.209  |
| H | 5.81683  | 2.64004  | -2.55709 | 250.5849 | 252.3661 | 253.8668 |
| H | 6.33927  | 3.79778  | -3.44779 | 255.0719 | 257.1549 | 257.9631 |
| O | 4.06555  | -1.55657 | -4.77046 | 259.5541 | 261.7917 | 263.536  |
| H | 3.56761  | -2.36288 | -5.05079 | 265.4023 | 267.9428 | 268.1278 |
| H | 3.76633  | -0.81870 | -5.34751 | 269.2491 | 270.5233 | 272.0396 |
| O | 6.29361  | -1.45500 | -3.21322 | 275.4403 | 277.9203 | 279.9837 |
| H | 5.51815  | -1.51006 | -3.82928 | 283.4096 | 284.0019 | 285.3732 |
| H | 7.07304  | -1.51377 | -3.77809 | 287.0592 | 287.2532 | 290.191  |
| O | 6.23832  | 1.07405  | -1.68283 | 291.4681 | 292.336  | 294.3322 |
| H | 6.71022  | 0.96707  | -0.82537 | 297.0639 | 299.3941 | 300.9475 |
| H | 6.32726  | 0.24058  | -2.18059 | 303.8555 | 305.6173 | 307.5897 |
| O | -4.95912 | -1.84756 | -5.03511 | 310.1806 | 313.6261 | 316.0686 |
| H | -5.58007 | -1.94517 | -5.76536 | 317.2922 | 319.0739 | 319.5182 |
| H | -4.76508 | -0.87912 | -4.96145 | 320.812  | 321.2521 | 323.6124 |
| O | -2.34166 | -3.21019 | -5.03770 | 324.907  | 327.1676 | 328.9266 |
| H | -3.21723 | -2.84084 | -5.25015 | 332.4419 | 335.4619 | 335.8574 |
| H | -2.00868 | -2.62533 | -4.31679 | 337.5576 | 338.9721 | 339.3047 |
| O | -4.20470 | 0.73549  | -4.55685 | 340.56   | 340.7545 | 343.8314 |
| H | -4.79986 | 1.50171  | -4.45300 | 344.1566 | 350.9358 | 353.3169 |
| H | -3.90300 | 0.54518  | -3.63782 | 354.6483 | 355.1504 | 358.4584 |
| O | 0.00322  | -2.53624 | -6.56111 | 360.079  | 361.6594 | 364.8751 |
| H | -0.82712 | -2.85282 | -6.15149 | 372.1365 | 372.792  | 374.2634 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | 0.73138  | -3.00309 | -6.11416 | 376.68   | 379.0655 | 379.9276 |
| O | 2.48715  | -3.72431 | -5.45898 | 384.4065 | 388.35   | 394.3473 |
| H | 2.35073  | -4.40641 | -4.73245 | 405.0037 | 431.8194 | 433.2021 |
| H | 2.78360  | -4.23338 | -6.22267 | 439.869  | 448.3925 | 457.9035 |
| O | -2.70786 | -5.73232 | -3.62693 | 458.7799 | 463.2574 | 467.1071 |
| H | -2.58981 | -4.92302 | -4.16346 | 468.9643 | 471.2536 | 473.344  |
| H | -3.33043 | -5.48484 | -2.92335 | 479.0791 | 484.4569 | 485.2538 |
| O | -0.24704 | -6.03278 | -2.30242 | 491.6421 | 498.4365 | 499.2854 |
| H | -1.06098 | -6.16578 | -2.83563 | 504.4649 | 513.173  | 515.0566 |
| H | -0.38316 | -5.12646 | -1.94486 | 518.0948 | 520.0673 | 521.5968 |
| O | 2.20631  | -5.60692 | -3.63160 | 533.2195 | 534.2781 | 536.5051 |
| H | 1.32400  | -5.80767 | -3.24604 | 538.8921 | 542.7965 | 545.4786 |
| H | 2.82151  | -5.55223 | -2.87806 | 546.3554 | 546.9796 | 548.992  |
| O | -6.71986 | 2.16479  | -1.31221 | 552.1867 | 556.0208 | 560.3497 |
| H | -6.43502 | 2.57809  | -0.47602 | 562.7353 | 565.2835 | 567.9285 |
| H | -6.77316 | 1.20336  | -1.15747 | 570.5474 | 574.2355 | 578.1278 |
| O | -7.12111 | -0.71400 | -0.88527 | 580.0054 | 583.4503 | 587.0034 |
| H | -6.91711 | -0.90362 | 0.06208  | 587.4044 | 591.951  | 597.2895 |
| H | -8.07401 | -0.83016 | -0.97715 | 598.5608 | 601.6737 | 606.3007 |
| O | -5.69036 | 3.05365  | -3.64059 | 607.7816 | 612.2927 | 613.4822 |
| H | -6.06467 | 2.73021  | -2.77802 | 615.4609 | 618.7529 | 620.5429 |
| H | -6.43039 | 3.43818  | -4.12309 | 623.8463 | 624.8468 | 626.1249 |
| O | -5.95772 | -2.86584 | -2.51713 | 629.7586 | 630.4426 | 634.7842 |
| H | -5.60562 | -2.49828 | -3.35110 | 635.0575 | 636.4953 | 638.1016 |
| H | -6.26532 | -2.11196 | -1.98210 | 640.2132 | 642.5457 | 642.9966 |
| O | -4.78193 | -5.07836 | -1.50468 | 645.4338 | 646.114  | 647.7284 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | -5.42786 | -5.75655 | -1.73481 | 652.1126 | 653.2129 | 653.8605 |
| H | -5.17807 | -4.22676 | -1.83295 | 655.1268 | 655.9932 | 658.246  |
| O | -6.26553 | -1.06644 | 1.67441  | 660.3481 | 662.3908 | 664.7204 |
| H | -6.12266 | -1.85935 | 2.22546  | 665.5452 | 668.7464 | 669.185  |
| H | -6.33621 | -0.26899 | 2.26608  | 670.6198 | 671.5768 | 673.5956 |
| O | -5.45277 | -3.47767 | 3.05826  | 674.7276 | 675.4788 | 677.0314 |
| H | -5.01071 | -4.04561 | 2.38334  | 679.3155 | 681.7222 | 683.0885 |
| H | -6.15701 | -4.01866 | 3.43412  | 684.9353 | 689.3202 | 690.5938 |
| O | -4.03597 | -4.93087 | 1.18666  | 693.6638 | 695.429  | 697.1169 |
| H | -4.30847 | -5.10002 | 0.25600  | 700.9276 | 701.5799 | 702.2341 |
| H | -3.40113 | -5.61894 | 1.47661  | 704.2132 | 704.9507 | 705.823  |
| O | 3.04007  | -6.41315 | 0.93143  | 710.7892 | 715.2832 | 716.0069 |
| H | 3.10042  | -5.90647 | 1.75781  | 718.3427 | 719.6911 | 721.1    |
| H | 2.09032  | -6.62989 | 0.79361  | 725.9112 | 727.8319 | 729.9218 |
| O | 0.36009  | -7.00593 | 0.34702  | 732.0757 | 735.0862 | 736.402  |
| H | -0.36977 | -6.70594 | 0.91171  | 742.525  | 743.9373 | 745.9679 |
| H | 0.10076  | -6.80119 | -0.57396 | 747.8069 | 751.7999 | 754.2469 |
| O | -1.89530 | -6.38608 | 2.28730  | 755.6515 | 758.0559 | 762.0417 |
| H | -1.98023 | -7.26988 | 2.66297  | 764.2906 | 769.273  | 773.8232 |
| H | -1.61471 | -5.79630 | 3.03336  | 776.1921 | 782.3818 | 784.3936 |
| O | 3.28973  | -4.54883 | 3.27017  | 790.0688 | 791.898  | 798.3821 |
| H | 2.71394  | -4.57391 | 4.06028  | 801.6296 | 803.1244 | 805.1295 |
| H | 4.12324  | -4.10512 | 3.52617  | 808.5067 | 812.9776 | 817.7766 |
| O | 6.71812  | -2.05048 | 1.46604  | 819.9406 | 821.3335 | 824.9837 |
| H | 6.46455  | -2.45155 | 0.61605  | 826.6531 | 834.8122 | 837.2979 |
| H | 6.77560  | -1.08628 | 1.31815  | 838.5026 | 840.4364 | 846.6505 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | 6.24884  | -3.40362 | -1.11547 | 848.1333  | 850.2528  | 851.4201  |
| H | 6.24612  | -2.76928 | -1.86410 | 857.0427  | 858.2274  | 861.376   |
| H | 7.05247  | -3.92680 | -1.22042 | 864.845   | 869.2506  | 873.9794  |
| O | 3.80667  | -5.10003 | -1.27523 | 876.6122  | 881.6181  | 886.8741  |
| H | 3.62353  | -5.62731 | -0.44910 | 893.5536  | 896.1154  | 897.2558  |
| H | 4.67852  | -4.68082 | -1.18316 | 898.3111  | 902.2029  | 903.4601  |
| O | 5.62267  | -2.95693 | 3.76169  | 907.0514  | 911.9527  | 917.7663  |
| H | 5.99365  | -2.62764 | 2.89918  | 918.2342  | 920.7184  | 924.4174  |
| H | 6.36549  | -3.36078 | 4.22423  | 927.2928  | 932.649   | 934.7573  |
| O | 4.98586  | 1.99268  | 4.96571  | 935.6959  | 939.0582  | 940.4358  |
| H | 4.77837  | 1.02793  | 4.97980  | 940.772   | 945.6669  | 952.2605  |
| H | 5.64590  | 2.14316  | 5.65122  | 957.6098  | 963.2813  | 969.4911  |
| O | 5.91201  | 2.64009  | 2.27364  | 971.3176  | 980.5439  | 982.8607  |
| H | 5.31889  | 3.30007  | 1.84650  | 986.5969  | 988.5603  | 993.0813  |
| H | 5.56683  | 2.46457  | 3.16816  | 995.7743  | 998.1643  | 1001.4238 |
| O | 7.13910  | 0.76073  | 0.91437  | 1003.3605 | 1006.9683 | 1009.5633 |
| H | 6.62498  | 1.45270  | 1.43671  | 1010.7103 | 1015.2881 | 1024.2066 |
| H | 8.06638  | 0.94252  | 1.10618  | 1031.1279 | 1037.1832 | 1042.3818 |
| O | 4.16005  | -0.62000 | 4.64731  | 1045.4892 | 1048.9747 | 1053.6207 |
| H | 3.87182  | -0.43878 | 3.72211  | 1060.9608 | 1065.8991 | 1071.3702 |
| H | 4.76652  | -1.37811 | 4.55128  | 1074.5149 | 1081.401  | 1089.0906 |
| O | -0.48342 | -0.01411 | 6.39532  | 1090.7884 | 1093.2659 | 1107.9725 |
| H | 0.33969  | -0.54825 | 6.46857  | 1112.5454 | 1159.488  | 1168.6144 |
| H | -0.25149 | 0.94311  | 6.56141  | 1641.5068 | 1643.6939 | 1645.4675 |
| O | -0.00063 | 2.60606  | 6.65406  | 1656.2648 | 1657.2003 | 1661.3339 |
| H | -0.75711 | 3.06622  | 6.23184  | 1662.7017 | 1662.9026 | 1663.6031 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | 0.80666  | 2.93219  | 6.21538  | 1664.9131 | 1665.1762 | 1665.9738 |
| O | 2.34145  | 3.33216  | 5.00129  | 1669.2779 | 1669.8239 | 1670.705  |
| H | 2.00929  | 2.68005  | 4.34351  | 1671.6635 | 1674.2534 | 1674.324  |
| H | 3.23107  | 3.00408  | 5.21811  | 1674.9961 | 1675.5135 | 1677.366  |
| O | 1.83717  | -1.57738 | 6.27165  | 1678.3477 | 1678.7911 | 1680.1904 |
| H | 1.67989  | -2.48457 | 5.95854  | 1680.5343 | 1680.9847 | 1681.9468 |
| H | 2.57492  | -1.22820 | 5.73852  | 1683.2202 | 1683.4949 | 1684.1852 |
| O | -1.12941 | -4.58240 | 4.23473  | 1684.7421 | 1686.1235 | 1686.3772 |
| H | -0.86637 | -3.82485 | 3.64678  | 1687.4658 | 1688.6648 | 1689.5158 |
| H | -1.92646 | -4.23442 | 4.70333  | 1691.7795 | 1692.7936 | 1693.5699 |
| O | -3.41470 | -3.39376 | 5.25419  | 1695.6218 | 1695.9451 | 1696.2864 |
| H | -3.30090 | -2.50444 | 5.64282  | 1697.1489 | 1698.3171 | 1700.4655 |
| H | -4.08231 | -3.30796 | 4.55202  | 1703.2078 | 1704.1803 | 1705.4477 |
| O | -3.07804 | -0.77159 | 6.46034  | 1705.6982 | 1707.2102 | 1707.8766 |
| H | -2.11992 | -0.53166 | 6.55002  | 1708.5698 | 1709.5655 | 1709.9777 |
| H | -3.43000 | -0.78290 | 7.35781  | 1710.7023 | 1712.4115 | 1712.8883 |
| O | 1.37471  | -4.39546 | 5.41597  | 1714.4117 | 1715.8733 | 1718.3714 |
| H | 0.45153  | -4.53073 | 5.08810  | 1719.9306 | 1720.9209 | 1722.6225 |
| H | 1.47142  | -4.97023 | 6.18364  | 1724.919  | 1726.3146 | 1726.7557 |
| O | 2.68200  | -0.96313 | -2.42761 | 1727.253  | 1728.0992 | 1730.5804 |
| H | 3.23600  | -1.18308 | -3.20618 | 1733.0478 | 1734.8007 | 1736.4401 |
| H | 1.87127  | -0.53462 | -2.82101 | 1740.678  | 1744.049  | 1745.8724 |
| O | 2.25355  | 2.96793  | -0.43861 | 1746.3082 | 1751.2358 | 1751.5998 |
| H | 2.69697  | 2.09332  | -0.38386 | 1754.7882 | 1755.8651 | 3010.7946 |
| H | 1.53346  | 3.00621  | 0.23903  | 3044.809  | 3110.9698 | 3132.6835 |
| O | -1.41549 | -1.62655 | -3.00332 | 3155.0107 | 3164.8869 | 3166.4937 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | -1.05257 | -2.30180 | -2.37439 | 3171.1615 | 3173.1499 | 3190.6437 |
| H | -0.68972 | -0.98370 | -3.18038 | 3194.3141 | 3203.8928 | 3208.2147 |
| O | -2.03944 | 2.55256  | -1.76367 | 3209.7899 | 3214.8572 | 3226.9812 |
| H | -1.08698 | 2.58429  | -2.03550 | 3239.6772 | 3246.5271 | 3249.0512 |
| H | -2.38686 | 1.64085  | -1.93093 | 3250.321  | 3253.6773 | 3254.4494 |
| O | 2.06856  | -2.62761 | 1.75977  | 3266.123  | 3266.4667 | 3270.5066 |
| H | 2.54002  | -3.34594 | 2.24364  | 3278.0245 | 3289.2309 | 3293.6291 |
| H | 2.12105  | -2.82247 | 0.78825  | 3295.7895 | 3298.6656 | 3301.9095 |
| O | 1.38744  | 1.53418  | 3.14943  | 3307.6429 | 3321.0248 | 3325.0873 |
| H | 2.05882  | 0.95316  | 2.72162  | 3326.5193 | 3334.2189 | 3339.6428 |
| H | 0.65087  | 0.92742  | 3.40822  | 3342.548  | 3349.2994 | 3359.0373 |
| O | -2.24221 | -2.87578 | 0.71444  | 3362.0578 | 3365.1108 | 3366.2511 |
| H | -2.83866 | -3.62399 | 0.93339  | 3372.9383 | 3374.1173 | 3375.7822 |
| H | -1.62208 | -2.74463 | 1.47844  | 3378.2351 | 3388.986  | 3396.5726 |
| O | -2.77583 | 0.92625  | 2.43767  | 3398.5998 | 3406.1778 | 3408.3015 |
| H | -2.58338 | 1.73220  | 1.89847  | 3413.9033 | 3418.7976 | 3423.5666 |
| H | -3.16319 | 0.29851  | 1.78153  | 3428.0194 | 3428.775  | 3432.0719 |
| O | -2.24324 | 3.00984  | 0.84699  | 3434.7646 | 3437.0906 | 3439.4874 |
| H | -2.81856 | 3.79450  | 0.98043  | 3441.7454 | 3448.1958 | 3448.7498 |
| H | -2.21425 | 2.82707  | -0.12906 | 3453.1358 | 3458.697  | 3462.0814 |
| O | -3.80153 | -0.67413 | 0.49247  | 3466.2262 | 3467.5811 | 3469.6403 |
| H | -3.26634 | -1.50356 | 0.55100  | 3475.2748 | 3479.3131 | 3480.279  |
| H | -4.69249 | -0.87587 | 0.85420  | 3484.3317 | 3484.8817 | 3490.6898 |
| O | -0.65701 | -0.11229 | 3.71878  | 3498.2439 | 3500.4889 | 3507.436  |
| H | -1.45620 | 0.30094  | 3.30779  | 3509.3386 | 3517.0126 | 3518.6289 |
| H | -0.71004 | -0.05731 | 4.70688  | 3520.0056 | 3521.8319 | 3523.4356 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| O | -0.53097 | -3.49268 | -1.31506 | 3532.6272 | 3533.4448 | 3538.8956 |
| H | 0.40952  | -3.33379 | -1.06074 | 3546.511  | 3546.8807 | 3549.6998 |
| H | -1.10765 | -3.33723 | -0.53245 | 3551.1712 | 3553.7264 | 3555.4718 |
| O | 3.20963  | -0.20569 | 2.11121  | 3561.7937 | 3563.0668 | 3568.3825 |
| H | 3.55390  | 0.08547  | 1.23941  | 3580.7351 | 3581.0227 | 3585.5884 |
| H | 2.78755  | -1.08648 | 1.95706  | 3586.9057 | 3587.4603 | 3594.0613 |
| O | 0.53403  | 2.68756  | -2.53094 | 3598.4015 | 3600.3381 | 3604.6883 |
| H | 0.73485  | 3.39417  | -3.19780 | 3608.1645 | 3619.3051 | 3623.0494 |
| H | 1.19421  | 2.81269  | -1.80469 | 3626.0151 | 3626.5541 | 3631.5462 |
| O | 0.36714  | 3.30423  | 1.42958  | 3632.3994 | 3635.4546 | 3646.4518 |
| H | 0.67091  | 2.65964  | 2.11670  | 3646.6885 | 3650.1171 | 3653.7084 |
| H | -0.58464 | 3.13537  | 1.23779  | 3655.3517 | 3655.9947 | 3658.2902 |
| O | -3.19331 | 0.13579  | -2.08826 | 3666.0624 | 3671.5949 | 3679.6122 |
| H | -2.56215 | -0.58616 | -2.34422 | 3682.2343 | 3688.3245 | 3691.4295 |
| H | -3.56580 | -0.11894 | -1.21596 | 3696.7152 | 3700.5551 | 3703.5475 |
| O | -0.45051 | -2.53688 | 2.65918  | 3703.824  | 3709.498  | 3710.4772 |
| H | 0.47263  | -2.58586 | 2.30242  | 3710.6892 | 3714.2247 | 3720.0508 |
| H | -0.52773 | -1.65087 | 3.10275  | 3722.3437 | 3723.2481 | 3725.6079 |
| O | 2.08575  | -3.06647 | -0.85863 | 3738.4141 | 3852.8693 | 3854.7742 |
| H | 2.69398  | -3.81867 | -1.07127 | 3855.5673 | 3856.4108 | 3857.4519 |
| H | 2.32626  | -2.31542 | -1.45404 | 3857.9735 | 3858.0851 | 3859.0776 |
| O | 3.72095  | 0.62467  | -0.48038 | 3859.1144 | 3859.6748 | 3860.9578 |
| H | 4.59109  | 0.87848  | -0.84741 | 3861.1568 | 3861.2998 | 3863.4614 |
| H | 3.33324  | 0.03572  | -1.17117 | 3863.6287 | 3864.257  | 3864.3514 |
| O | 0.55733  | 0.17761  | -3.49708 | 3867.0885 | 3867.9718 | 3870.3909 |
| H | 0.53779  | 0.19168  | -4.48914 |           |           |           |

|                                   |   |          |          |          |         |         |         |
|-----------------------------------|---|----------|----------|----------|---------|---------|---------|
|                                   | H | 0.53588  | 1.11764  | -3.18489 |         |         |         |
| (H <sub>2</sub> O) <sub>100</sub> | O | 0.10401  | -0.06225 | 7.79992  | 31.8189 | 32.8069 | 33.5923 |
|                                   | O | 5.20385  | -0.00021 | 4.01101  | 33.8296 | 34.6452 | 35.4437 |
|                                   | O | -5.81659 | 3.75430  | 3.84337  | 35.714  | 35.8046 | 36.0337 |
|                                   | O | -0.77581 | 2.10824  | 3.10624  | 36.6454 | 40.9946 | 41.2992 |
|                                   | O | -2.41132 | -3.81681 | 6.48782  | 41.7534 | 43.5087 | 45.0945 |
|                                   | O | -1.17499 | -0.58057 | 3.60500  | 46.4519 | 47.0138 | 47.1883 |
|                                   | O | 6.46989  | -2.56517 | 3.81399  | 47.2008 | 47.3622 | 48.054  |
|                                   | O | -3.99839 | 2.94564  | 5.94648  | 48.5441 | 49.0262 | 49.4191 |
|                                   | O | 3.02983  | 0.00337  | 2.32224  | 49.7753 | 49.8998 | 50.9811 |
|                                   | O | 1.19298  | -1.87739 | 3.14445  | 51.1076 | 51.2787 | 51.8076 |
|                                   | O | 0.11673  | -5.10846 | 5.91289  | 52.0311 | 52.4787 | 52.7879 |
|                                   | O | -6.29735 | -0.49356 | 4.66186  | 53.0541 | 53.2696 | 53.4391 |
|                                   | O | 7.05631  | -3.15060 | 1.34325  | 53.8982 | 54.2281 | 55.278  |
|                                   | O | 2.11486  | -3.20992 | 5.39971  | 56.5165 | 56.917  | 58.3386 |
|                                   | O | 2.34050  | -1.31014 | 7.38184  | 59.7595 | 59.9084 | 61.1567 |
|                                   | O | 3.11637  | 3.04624  | 6.53628  | 62.1013 | 62.8934 | 62.9808 |
|                                   | O | 3.16737  | 4.17774  | 3.99886  | 63.3115 | 63.6591 | 64.4038 |
|                                   | O | -5.16818 | -2.58505 | 3.17510  | 64.8317 | 64.8366 | 65.1981 |
|                                   | O | 0.38585  | 2.61188  | 7.37081  | 65.3547 | 66.0034 | 66.2646 |
|                                   | O | -4.19850 | -4.79658 | 4.67062  | 66.4834 | 66.6618 | 66.7785 |
|                                   | O | -6.48415 | 1.05406  | 0.38194  | 67.3602 | 67.8289 | 69.8367 |
|                                   | O | -7.15222 | 1.46780  | 3.14793  | 70.0146 | 72.6579 | 72.9304 |
|                                   | O | 3.78738  | -0.57717 | -0.24594 | 73.2737 | 73.5761 | 74.0111 |
|                                   | O | 4.61919  | -4.34182 | 4.73027  | 74.1205 | 74.8523 | 74.8647 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | -4.39890 | 0.43551  | 6.54594  | 75.1891  | 76.1062  | 76.5087  |
| O | 4.23837  | 0.65647  | 6.55119  | 76.7086  | 77.4064  | 77.8237  |
| O | -3.05639 | -1.51898 | 1.84813  | 78.7163  | 78.7698  | 79.8146  |
| O | -2.05092 | -1.02188 | 6.18574  | 80.536   | 80.6986  | 81.5842  |
| O | -1.77233 | -7.52830 | -1.28030 | 82.2989  | 82.7351  | 84.6791  |
| O | 4.17457  | -4.78601 | -1.77244 | 84.7814  | 86.4428  | 86.7693  |
| O | -6.92542 | -2.05074 | -3.07155 | 87.4526  | 88.4597  | 88.7434  |
| O | -1.82579 | -2.46210 | -2.33384 | 88.8381  | 89.4979  | 89.5587  |
| O | -2.97036 | -6.44894 | 3.11638  | 90.7217  | 91.0962  | 91.4237  |
| O | -1.80687 | -3.40216 | 0.25048  | 92.9366  | 93.5034  | 93.529   |
| O | 5.67887  | -5.47910 | 0.47455  | 94.5766  | 96.0942  | 97.1724  |
| O | -5.76874 | -4.38339 | -3.06022 | 97.4106  | 97.8368  | 98.3081  |
| O | 2.40153  | -2.80300 | -1.02936 | 98.5832  | 99.0734  | 100.1982 |
| O | 0.79971  | -3.59408 | 1.06265  | 101.4643 | 102.3295 | 102.6858 |
| O | -0.27824 | -6.81628 | 3.92234  | 102.8169 | 104.0704 | 104.2336 |
| O | -6.93907 | -3.45566 | 1.28642  | 106.4254 | 106.6331 | 106.8619 |
| O | 1.45947  | -6.17024 | 1.78533  | 112.6567 | 114.1932 | 115.1714 |
| O | 1.00675  | -7.77890 | -0.53986 | 117.4167 | 117.632  | 118.0043 |
| O | 0.93198  | -6.24858 | -4.65311 | 118.1077 | 120.4539 | 122.2549 |
| O | 1.39058  | -3.57998 | -5.36403 | 122.7854 | 123.9403 | 124.2499 |
| O | -1.73809 | -6.59431 | -3.74847 | 125.3241 | 130.5434 | 135.8589 |
| O | -7.73729 | -1.34281 | -0.53325 | 137.3497 | 139.1939 | 139.9059 |
| O | 4.12148  | -6.10981 | 2.48765  | 144.2711 | 144.8498 | 145.6596 |
| O | -5.62845 | -5.37350 | -0.39824 | 147.5379 | 148.4991 | 148.9119 |
| O | 2.50349  | -6.94009 | -2.67927 | 149.95   | 151.0635 | 152.4396 |
| O | -3.10253 | -5.79290 | 0.44261  | 152.9919 | 153.7756 | 158.7166 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | 1.77233  | 7.52830  | 1.28030  | 160.5129 | 161.998  | 163.238  |
| O | -4.17457 | 4.78601  | 1.77244  | 165.0429 | 165.3839 | 165.5459 |
| O | 6.92542  | 2.05074  | 3.07155  | 165.9737 | 168.4253 | 172.2847 |
| O | 1.82579  | 2.46210  | 2.33384  | 172.3334 | 174.3389 | 174.9593 |
| O | 2.97036  | 6.44894  | -3.11638 | 177.3985 | 177.9419 | 178.6096 |
| O | 1.80687  | 3.40216  | -0.25048 | 179.0127 | 180.1982 | 181.544  |
| O | -5.67887 | 5.47910  | -0.47455 | 183.1133 | 184.4324 | 184.9263 |
| O | 5.76874  | 4.38339  | 3.06022  | 184.9987 | 185.6475 | 187.783  |
| O | -2.40153 | 2.80300  | 1.02936  | 190.506  | 191.1943 | 192.3508 |
| O | -0.79971 | 3.59408  | -1.06265 | 193.551  | 194.0566 | 194.807  |
| O | 0.27824  | 6.81628  | -3.92234 | 196.9399 | 197.5822 | 198.0475 |
| O | 6.93907  | 3.45566  | -1.28642 | 198.4694 | 200.887  | 201.2813 |
| O | -7.05631 | 3.15060  | -1.34325 | 202.6684 | 203.1617 | 204.0717 |
| O | -1.45947 | 6.17024  | -1.78533 | 204.6604 | 206.881  | 207.6205 |
| O | -1.00675 | 7.77890  | 0.53986  | 208.2309 | 209.1128 | 210.9301 |
| O | -0.93198 | 6.24858  | 4.65311  | 211.3396 | 212.8567 | 214.4078 |
| O | -1.39058 | 3.57998  | 5.36403  | 215.336  | 215.3742 | 215.7827 |
| O | 5.16818  | 2.58505  | -3.17510 | 218.551  | 219.3732 | 221.8732 |
| O | 1.73809  | 6.59431  | 3.74847  | 223.0073 | 223.2931 | 224.8121 |
| O | 4.19850  | 4.79658  | -4.67062 | 225.1957 | 226.7256 | 226.7433 |
| O | 6.48415  | -1.05406 | -0.38194 | 227.6571 | 230.0197 | 232.4696 |
| O | 7.73729  | 1.34281  | 0.53325  | 232.4959 | 234.512  | 234.855  |
| O | -3.78738 | 0.57717  | 0.24594  | 238.2014 | 240.7478 | 242.6443 |
| O | -4.12148 | 6.10981  | -2.48765 | 245.3848 | 246.5423 | 246.6716 |
| O | 5.62845  | 5.37350  | 0.39824  | 249.2109 | 249.5195 | 250.9614 |
| O | -2.50349 | 6.94009  | 2.67927  | 252.5678 | 252.723  | 253.1599 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| O | 3.05639  | 1.51898  | -1.84813 | 256.4173 | 256.9233 | 257.4389 |
| O | 3.10253  | 5.79290  | -0.44261 | 258.5702 | 259.7739 | 261.1805 |
| O | -0.10401 | 0.06225  | -7.79992 | 261.4532 | 262.0671 | 264.5816 |
| O | -5.20385 | 0.00021  | -4.01101 | 264.8277 | 265.6587 | 266.1551 |
| O | 5.81659  | -3.75430 | -3.84337 | 268.3535 | 268.6025 | 268.9321 |
| O | 0.77581  | -2.10824 | -3.10624 | 272.1939 | 274.6264 | 275.516  |
| O | 2.41132  | 3.81681  | -6.48782 | 277.7743 | 278.1833 | 281.904  |
| O | 1.17499  | 0.58057  | -3.60500 | 282.6295 | 283.8455 | 285.7902 |
| O | -6.46989 | 2.56517  | -3.81399 | 287.3651 | 291.1518 | 296.4265 |
| O | 3.99839  | -2.94564 | -5.94648 | 299.3482 | 299.7473 | 302.0221 |
| O | -3.02983 | -0.00337 | -2.32224 | 303.7024 | 304.3933 | 306.5702 |
| O | -1.19298 | 1.87739  | -3.14445 | 307.0141 | 308.4409 | 308.8915 |
| O | -0.11673 | 5.10846  | -5.91289 | 312.1171 | 314.0637 | 316.6524 |
| O | 6.29735  | 0.49356  | -4.66186 | 317.433  | 318.086  | 319.2833 |
| O | -2.11486 | 3.20992  | -5.39971 | 322.5006 | 324.571  | 325.7515 |
| O | -2.34050 | 1.31014  | -7.38184 | 326.0205 | 327.0243 | 327.2492 |
| O | -3.11637 | -3.04624 | -6.53628 | 327.9828 | 328.3517 | 328.9201 |
| O | -3.16737 | -4.17774 | -3.99886 | 329.6968 | 330.6302 | 330.6921 |
| O | -0.38585 | -2.61188 | -7.37081 | 331.9313 | 331.9435 | 342.3752 |
| O | 7.15222  | -1.46780 | -3.14793 | 342.9848 | 346.0283 | 346.0819 |
| O | -4.61919 | 4.34182  | -4.73027 | 346.9178 | 347.0846 | 349.3721 |
| O | 4.39890  | -0.43551 | -6.54594 | 349.3946 | 354.5795 | 355.2098 |
| O | -4.23837 | -0.65647 | -6.55119 | 355.9949 | 356.7579 | 357.9195 |
| O | 2.05092  | 1.02188  | -6.18574 | 358.3935 | 366.28   | 366.3039 |
| H | 2.35972  | -0.64982 | 2.63319  | 368.5084 | 368.6523 | 372.5055 |
| H | 2.59462  | 0.89061  | 2.34079  | 372.9518 | 376.1058 | 376.317  |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | 2.27958  | 2.75566  | -0.82458 | 381.9472 | 381.976  | 386.8716 |
| H | 2.28740  | 4.26464  | -0.32760 | 387.3709 | 390.8057 | 390.926  |
| H | 1.82689  | -2.57891 | -1.80275 | 392.2075 | 392.2093 | 397.1455 |
| H | 3.01474  | -3.51834 | -1.31804 | 397.342  | 398.6885 | 398.7291 |
| H | 0.32440  | 1.06816  | -3.48330 | 402.5265 | 402.5293 | 409.6932 |
| H | 1.46651  | 0.73938  | -4.53257 | 409.7272 | 415.7629 | 415.7749 |
| H | -0.32440 | -1.06816 | 3.48330  | 460.004  | 460.1076 | 475.2416 |
| H | -1.46651 | -0.73938 | 4.53257  | 475.293  | 482.3873 | 482.4474 |
| H | -1.82689 | 2.57891  | 1.80275  | 492.1427 | 492.2516 | 496.7907 |
| H | -3.01474 | 3.51834  | 1.31804  | 496.8579 | 498.5933 | 498.6427 |
| H | -2.27958 | -2.75566 | 0.82458  | 500.5326 | 500.5895 | 508.2216 |
| H | -2.28740 | -4.26464 | 0.32760  | 508.253  | 512.5106 | 512.5308 |
| H | -2.35972 | 0.64982  | -2.63319 | 514.2049 | 514.2896 | 514.8645 |
| H | -2.59462 | -0.89061 | -2.34079 | 515.007  | 527.2103 | 527.2143 |
| H | -1.05943 | 2.52864  | -2.41130 | 562.5063 | 562.8662 | 565.6128 |
| H | -1.52567 | 2.37602  | -3.92513 | 565.9205 | 568.4376 | 568.503  |
| H | -1.84682 | -2.83838 | -1.42138 | 572.825  | 572.8851 | 576.0966 |
| H | -2.31562 | -3.09017 | -2.91898 | 576.2603 | 584.0054 | 584.2367 |
| H | -3.28844 | 1.38612  | 0.51689  | 592.512  | 592.523  | 594.7396 |
| H | -3.51287 | 0.37757  | -0.68261 | 594.7948 | 599.5333 | 600.0456 |
| H | 1.36179  | -3.32708 | 0.29625  | 603.5919 | 604.1485 | 610.2392 |
| H | -0.13881 | -3.53970 | 0.75715  | 610.8355 | 614.8133 | 615.757  |
| H | -0.88761 | 1.14886  | 3.30256  | 617.095  | 617.4565 | 621.9882 |
| H | 0.16893  | 2.23804  | 2.84683  | 622.123  | 625.6351 | 626.2029 |
| H | 2.38139  | 1.17139  | -2.48071 | 627.7548 | 628.1321 | 629.1197 |
| H | 3.32221  | 0.75655  | -1.27667 | 629.2282 | 633.1957 | 633.5639 |

|   |          |          |          |          |          |          |
|---|----------|----------|----------|----------|----------|----------|
| H | 0.13881  | 3.53970  | -0.75715 | 635.2645 | 635.8643 | 638.2767 |
| H | -1.36179 | 3.32708  | -0.29625 | 638.7006 | 641.1652 | 642.7655 |
| H | 0.88761  | -1.14886 | -3.30256 | 643.4682 | 643.9542 | 645.0252 |
| H | -0.16893 | -2.23804 | -2.84683 | 646.0864 | 648.7869 | 650.2937 |
| H | -2.38139 | -1.17139 | 2.48071  | 650.4077 | 652.0679 | 653.6869 |
| H | -3.32221 | -0.75655 | 1.27667  | 653.8525 | 655.2689 | 655.5258 |
| H | 1.05943  | -2.52864 | 2.41130  | 657.8986 | 658.8347 | 661.2175 |
| H | 1.52567  | -2.37602 | 3.92513  | 664.2961 | 665.95   | 667.2504 |
| H | 1.84682  | 2.83838  | 1.42138  | 667.8919 | 670.071  | 671.8392 |
| H | 2.31562  | 3.09017  | 2.91898  | 672.3431 | 674.2977 | 675.5976 |
| H | 3.51287  | -0.37757 | 0.68261  | 676.3666 | 676.4549 | 676.4976 |
| H | 3.28844  | -1.38612 | -0.51689 | 677.6879 | 677.8317 | 680.1166 |
| H | -1.15581 | 7.25649  | -0.27248 | 680.4913 | 680.5364 | 683.2136 |
| H | -0.05910 | 7.68476  | 0.75148  | 685.5705 | 686.9529 | 691.0145 |
| H | -1.14757 | 3.07286  | 4.55505  | 691.2483 | 694.1865 | 696.6994 |
| H | -1.24379 | 4.52653  | 5.14513  | 697.6618 | 701.0749 | 706.352  |
| H | 4.94083  | 5.30183  | -5.02189 | 706.9441 | 707.091  | 707.8961 |
| H | 3.70806  | 5.43251  | -4.04414 | 709.7699 | 709.9631 | 711.9064 |
| H | -3.16130 | 6.14692  | -2.26612 | 712.9977 | 715.2664 | 717.3052 |
| H | -4.21834 | 5.49542  | -3.23711 | 718.4662 | 720.9092 | 724.9928 |
| H | -4.54946 | 3.24609  | 5.20189  | 726.5531 | 728.8706 | 731.8552 |
| H | -3.06847 | 3.20817  | 5.74355  | 732.5438 | 734.3751 | 737.1452 |
| H | 2.03016  | 6.59291  | -3.34463 | 742.3014 | 745.1696 | 746.4866 |
| H | 3.01283  | 6.25412  | -2.15037 | 747.1324 | 754.4832 | 754.5069 |
| H | -6.24110 | 6.24898  | -0.33268 | 756.865  | 758.2053 | 761.0896 |
| H | -5.06562 | 5.72607  | -1.23376 | 762.479  | 767.0044 | 769.1737 |

|   |          |         |          |          |          |          |
|---|----------|---------|----------|----------|----------|----------|
| H | 0.69976  | 4.61047 | -6.10029 | 769.9979 | 772.5719 | 777.8315 |
| H | -0.82419 | 4.44583 | -5.75814 | 778.814  | 781.7434 | 783.3808 |
| H | -4.70651 | 0.44417 | 7.45945  | 783.9487 | 784.2705 | 785.9462 |
| H | -4.21892 | 1.40062 | 6.31186  | 789.5586 | 792.0893 | 793.7228 |
| H | -4.78871 | 4.44948 | 2.45457  | 794.7575 | 799.0736 | 801.4011 |
| H | -4.72221 | 5.04849 | 0.99994  | 802.2581 | 805.724  | 806.1228 |
| H | -3.08564 | 6.22296 | 2.36498  | 809.2326 | 809.3064 | 816.9306 |
| H | -1.99090 | 7.25062 | 1.89277  | 818.2005 | 820.759  | 822.7326 |
| H | 0.82851  | 6.44354 | 4.07658  | 825.1156 | 827.5627 | 831.4561 |
| H | 2.23021  | 5.75637 | 3.87528  | 832.6044 | 835.4296 | 837.9495 |
| H | 3.18581  | 3.80051 | 4.90697  | 840.9617 | 843.6053 | 848.0225 |
| H | 4.10392  | 4.26236 | 3.70783  | 849.739  | 851.1991 | 852.157  |
| H | -3.00421 | 3.57692 | -5.21910 | 857.0002 | 857.5445 | 858.6838 |
| H | -2.21738 | 2.55299 | -6.12876 | 860.1099 | 861.143  | 862.8192 |
| H | 2.15995  | 8.40862 | 1.34033  | 864.7812 | 864.8529 | 868.7163 |
| H | 1.76665  | 7.16571 | 2.21653  | 869.0264 | 869.1479 | 870.2703 |
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| H | -5.32239 | 3.70500 | -4.44359 | 877.5177 | 880.2423 | 881.6798 |
| H | 2.24000  | 1.97188 | -6.31899 | 883.3531 | 883.5601 | 886.7086 |
| H | 2.88786  | 0.53207 | -6.34648 | 887.127  | 892.4196 | 892.7858 |
| H | 3.08742  | 4.19440 | -5.87031 | 894.2805 | 894.6871 | 901.6508 |
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| H | -6.35489 | 2.96042 | 3.60279  | 908.1015 | 908.7755 | 916.7487 |
| H | -6.42307 | 4.38856 | 4.24203  | 917.4045 | 919.5162 | 923.2088 |
| H | 0.12241  | 7.70209 | -4.26880 | 924.6298 | 928.2812 | 929.4253 |
| H | 0.10609  | 6.18331 | -4.67808 | 929.5202 | 935.3925 | 937.0098 |

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| H | -1.54270 | 6.51133  | 3.89339  | 941.3809  | 942.4602  | 947.8414  |
| H | -1.10992 | 6.87345  | 5.36508  | 948.3765  | 951.2302  | 952.7782  |
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| H | -1.28963 | -2.79547 | -7.05364 | 1050.7193 | 1052.9806 | 1070.3608 |
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| H | -5.64589 | -0.20073 | 5.33152  | 1110.4741 | 1113.5389 | 1117.2733 |
| H | -3.55210 | -2.14177 | -6.53884 | 1156.2102 | 1156.3161 | 1159.8151 |
| H | -3.55849 | -3.55722 | -7.22336 | 1159.8586 | 1161.8095 | 1161.8443 |
| H | -6.86956 | 2.42671  | -0.70335 | 1166.468  | 1166.5416 | 1175.0952 |
| H | -6.60045 | 3.94911  | -1.01046 | 1175.1752 | 1199.9597 | 1199.9816 |
| H | -2.59310 | 1.64838  | -8.24830 | 1660.3803 | 1660.3903 | 1660.6103 |
| H | -1.46201 | 0.82348  | -7.52539 | 1660.7582 | 1663.2574 | 1663.3451 |
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| H | -5.51157 | 0.88580  | 0.34128  | 1666.0585 | 1666.1615 | 1666.2546 |
| H | -7.33179 | -0.50932 | -0.22216 | 1666.753  | 1666.842  | 1668.2477 |
| H | -7.44748 | -2.02848 | 0.09481  | 1668.3092 | 1669.52   | 1669.5801 |
| H | -5.68342 | -5.01854 | -1.30853 | 1672.6577 | 1672.7266 | 1673.3427 |
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| H | -2.67458 | -6.43823 | -0.16350 | 1678.4665 | 1678.5604 | 1679.5297 |
| H | -4.03468 | -5.66699 | 0.12008  | 1680.8354 | 1681.0986 | 1681.135  |
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| H | -6.34320 | -4.96016 | -3.57617 | 1686.966  | 1687.5301 | 1688.1551 |
| H | -0.17535 | -0.91443 | -7.64882 | 1690.197  | 1690.3125 | 1690.7474 |
| H | 0.64964  | 0.37499  | -7.26441 | 1691.0907 | 1691.2368 | 1691.344  |
| H | -6.81793 | 0.70631  | 3.71868  | 1692.6929 | 1692.837  | 1692.9654 |
| H | -8.11370 | 1.44695  | 3.21611  | 1694.183  | 1694.8661 | 1695.7043 |
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| H | -4.59662 | -0.39314 | -5.67555 | 1701.3041 | 1701.8281 | 1703.7022 |
| H | -7.72985 | -3.77228 | 1.73670  | 1704.5847 | 1704.9769 | 1705.1297 |
| H | -6.31678 | -3.14856 | 1.99274  | 1705.9255 | 1707.1187 | 1707.7377 |
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| H | -5.63327 | 0.87397  | -3.92774 | 1711.3481 | 1711.6356 | 1711.9144 |
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| H | 3.55849  | 3.55722  | 7.22336  | 1739.8713 | 1739.9116 | 1743.3768 |
| H | 3.55210  | 2.14177  | 6.53884  | 1745.2468 | 2812.5918 | 2813.4535 |

|   |          |          |          |           |           |           |
|---|----------|----------|----------|-----------|-----------|-----------|
| H | 6.86956  | -2.42671 | 0.70335  | 2878.9833 | 2880.1524 | 2917.0472 |
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| H | 2.59310  | -1.64838 | 8.24830  | 2968.2945 | 3002.9063 | 3004.8924 |
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| H | 4.70651  | -0.44417 | -7.45945 | 3069.8937 | 3080.8019 | 3081.2279 |
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| H | 5.68342  | 5.01854  | 1.30853  | 3289.7663 | 3296.7185 | 3304.5314 |
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| H | 6.34320  | 4.96016  | 3.57617  | 3344.0946 | 3344.484  | 3344.9926 |
| H | 6.21358  | 3.47393  | 3.06376  | 3348.3775 | 3353.6595 | 3355.0068 |
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| H | -0.64964 | -0.37499 | 7.26441  | 3411.0648 | 3412.7499 | 3412.9225 |
| H | 6.81793  | -0.70631 | -3.71868 | 3424.2361 | 3424.2719 | 3427.6416 |
| H | 8.11370  | -1.44695 | -3.21611 | 3429.1582 | 3436.6539 | 3439.6964 |

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| H | 4.59662  | 0.39314  | 5.67555  | 3444.6266 | 3447.3683 | 3448.9072 |
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| H | 5.63327  | -0.87397 | 3.92774  | 3474.4888 | 3474.8147 | 3477.8687 |
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| H | 3.16130  | -6.14692 | 2.26612  | 3541.0288 | 3549.8588 | 3550.0589 |
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| H | 3.06847  | -3.20817 | -5.74355 | 3564.094  | 3567.5989 | 3568.0493 |
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| H | -2.03016 | -6.59291 | 3.34463  | 3572.75   | 3574.6955 | 3575.0596 |
| H | 5.06562  | -5.72607 | 1.23376  | 3578.9323 | 3579.2108 | 3583.2451 |
| H | 6.24110  | -6.24898 | 0.33268  | 3583.3545 | 3587.8413 | 3588.5253 |
| H | -0.69976 | -4.61047 | 6.10029  | 3591.9373 | 3592.0522 | 3594.3158 |
| H | 0.82419  | -4.44583 | 5.75814  | 3594.7973 | 3597.0499 | 3597.3646 |
| H | 4.72221  | -5.04849 | -0.99994 | 3598.1499 | 3598.3524 | 3615.9174 |
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| H | 3.08564  | -6.22296 | -2.36498 | 3628.0065 | 3628.1138 | 3633.4703 |
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| H | -0.82851 | -6.44354 | -4.07658 | 3646.564  | 3646.6861 | 3647.5292 |
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| H | -2.65927 | -4.10183 | 7.37463  | 3860.048  | 3860.6711 | 3860.6744 |
| H | 6.42307  | -4.38856 | -4.24203 | 3861.2629 | 3861.2635 | 3861.3123 |
| H | 6.35489  | -2.96042 | -3.60279 | 3861.3226 | 3862.4042 | 3862.4087 |
| H | -0.12241 | -7.70209 | 4.26880  | 3863.0454 | 3863.0493 | 3863.1933 |
| H | -0.10609 | -6.18331 | 4.67808  | 3863.1999 | 3863.3354 | 3863.3746 |
| H | 1.10992  | -6.87345 | -5.36508 | 3864.0079 | 3864.029  | 3864.6373 |
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| H | 0.86635  | -6.42125 | 2.52286  |           |           |           |
| H | 1.19708  | -5.25657 | 1.52278  |           |           |           |

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