SUPPLEMENTARY MATERIAL

On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water

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Tabel S1: HF: shieldings and shielding anisotropies

| Basis sets | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|-----------------------------|---------------------------|
|            | Shielding                   | Anisotropy                | Shielding | Anisotropy |
|            | O   | H   | O   | H   | O   | H   | O   | H   |
| pVDZ       | 347.957 | 31.380 | 30.588 | 19.730 | 353.748 | 31.817 | 30.163 | 20.332 |
| pVTZ       | 335.625 | 30.836 | 42.408 | 20.709 | 343.690 | 31.457 | 41.938 | 21.581 |
| pVQZ       | 331.477 | 30.609 | 51.084 | 20.853 | 340.135 | 31.241 | 50.488 | 21.795 |
| pV5Z       | 328.635 | 30.506 | 55.182 | 20.919 | 337.360 | 31.128 | 54.612 | 21.868 |
| pV6Z       | 327.957 | 30.481 | 56.718 | 20.939 | 336.738 | 31.101 | 56.059 | 21.888 |
| aug-pVDZ   | 337.262 | 31.199 | 51.075 | 19.766 | 343.918 | 31.672 | 50.520 | 20.487 |
| aug-pVTZ   | 328.803 | 30.751 | 56.138 | 20.587 | 336.700 | 31.335 | 55.657 | 21.425 |
| aug-pVQZ   | 328.577 | 30.564 | 56.793 | 20.820 | 337.180 | 31.128 | 56.123 | 21.749 |
| aug-pV5Z   | 327.909 | 30.505 | 57.255 | 20.907 | 336.662 | 31.125 | 56.569 | 21.852 |
| aug-pV6Z   | 327.847 | 30.479 | 57.325 | 20.944 | 336.619 | 31.099 | 56.641 | 21.892 |
| aug-pc-1   | 335.256 | 31.012 | 51.651 | 19.994 | 341.842 | 31.456 | 51.142 | 20.659 |
| aug-pc-2   | 326.211 | 30.668 | 57.361 | 20.698 | 335.247 | 31.300 | 56.688 | 21.635 |
| aug-pc-3   | 327.423 | 30.491 | 57.646 | 20.929 | 336.261 | 31.112 | 56.959 | 21.878 |
| aug-pc-4   | 327.861 | 30.468 | 57.318 | 20.961 | 336.633 | 31.087 | 56.633 | 21.911 |
| aug-pcS-1  | 326.009 | 30.521 | 58.403 | 20.531 | 332.390 | 30.938 | 58.220 | 21.202 |
| aug-pcS-2  | 329.281 | 30.557 | 57.748 | 20.843 | 338.130 | 31.177 | 57.044 | 21.795 |
| aug-pcS-3  | 327.848 | 30.466 | 57.365 | 20.962 | 336.617 | 31.084 | 56.675 | 21.913 |
| aug-pcS-4  | 327.846 | 30.465 | 57.327 | 20.965 | 336.625 | 31.084 | 56.641 | 21.916 |
| Basis sets | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|-------------------------------|--------------------------|
|            | Shielding | Anisotropy | Shielding | Anisotropy |
|            | O   | H    | O   | H    | O   | H    | O   | H    | O   | H    | O   | H    |
| pVDZ       | 345.491 | 31.915 | 24.569 | 18.308 | 338.590 | 31.605 | 24.218 | 17.634 |
| pVTZ       | 336.094 | 31.480 | 35.247 | 19.460 | 333.773 | 31.314 | 35.292 | 19.224 |
| pVQZ       | 331.541 | 31.218 | 45.936 | 19.652 | 329.821 | 31.075 | 46.070 | 19.476 |
| pV5Z       | 328.142 | 31.067 | 51.648 | 19.749 | 326.409 | 30.910 | 51.842 | 19.574 |
| pV6Z       | 326.961 | 31.038 | 54.245 | 19.756 | 325.190 | 30.878 | 54.460 | 19.579 |
| aug-pVDZ   | 336.410 | 31.649 | 50.225 | 18.573 | 332.335 | 31.342 | 50.340 | 18.143 |
| aug-pVTZ   | 328.345 | 31.306 | 53.985 | 19.412 | 325.798 | 31.082 | 54.195 | 19.157 |
| aug-pVQZ   | 327.851 | 31.123 | 54.895 | 19.639 | 325.943 | 30.950 | 55.113 | 19.447 |
| aug-pV5Z   | 326.962 | 31.058 | 55.523 | 19.732 | 325.136 | 30.893 | 55.745 | 19.549 |
| aug-pV6Z   | 326.795 | 31.033 | 55.649 | 19.767 | 324.991 | 30.869 | 55.870 | 19.586 |
| aug-pc-1   | 335.158 | 31.463 | 49.819 | 18.829 | 330.237 | 31.103 | 49.979 | 18.336 |
| aug-pc-2   | 326.407 | 31.218 | 55.282 | 19.492 | 324.318 | 31.035 | 55.535 | 19.287 |
| aug-pc-3   | 326.619 | 31.045 | 55.690 | 19.749 | 324.802 | 30.881 | 55.916 | 19.568 |
| aug-pc-4   | 326.737 | 31.021 | 55.679 | 19.784 | 324.930 | 30.858 | 55.904 | 19.604 |
| aug-pcS-1  | 325.970 | 31.065 | 57.241 | 19.311 | 321.596 | 30.745 | 57.524 | 18.861 |
| aug-pcS-2  | 328.422 | 31.106 | 56.136 | 19.654 | 326.578 | 30.935 | 56.370 | 19.472 |
| aug-pcS-3  | 326.747 | 31.022 | 55.688 | 19.783 | 324.940 | 30.859 | 55.909 | 19.602 |
| aug-pcS-4  | 326.753 | 31.018 | 55.668 | 19.788 | 324.955 | 30.855 | 55.890 | 19.609 |
| Basis sets   | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|-------------|-----------------------------|---------------------------|
|             | Shielding                  | Anisotropy                | Shielding                  | Anisotropy                |
|             | O  | H  | O  | H  | O  | H  | O  | H  | O  | H  | O  | H  |
| pVDZ        | 363.215 | 31.602 | 17.982 | 19.531 | 360.091 | 31.474 | 17.622 | 19.131 |
| pVTZ        | 352.760 | 31.002 | 28.654 | 20.602 | 352.132 | 30.994 | 28.376 | 20.509 |
| pVQZ        | 349.399 | 30.628 | 37.754 | 20.896 | 349.263 | 30.643 | 37.645 | 20.873 |
| pV5Z        | 346.870 | 30.456 | 42.337 | 21.018 | 346.603 | 30.443 | 42.274 | 20.979 |
| pV6Z        | 346.141 | 30.410 | 44.413 | 21.051 | 345.782 | 30.385 | 44.363 | 21.001 |
| aug-pVDZ    | 353.889 | 31.682 | 40.743 | 20.595 | 344.862 | 30.658 | 44.029 | 20.385 |
| aug-pVTZ    | 346.459 | 30.523 | 44.880 | 20.916 | 345.825 | 30.473 | 44.813 | 20.830 |
| aug-pVQZ    | 346.022 | 30.435 | 45.412 | 21.026 | 345.571 | 30.400 | 45.265 | 20.965 |
| aug-pV6Z    | 346.054 | 30.397 | 45.363 | 21.073 | 345.606 | 30.361 | 45.321 | 21.012 |
| pCVDZ       | 362.085 | 31.591 | 18.041 | 19.531 | 359.307 | 31.488 | 17.621 | 19.173 |
| pCVTZ       | 352.852 | 30.960 | 30.205 | 20.602 | 352.653 | 30.990 | 30.009 | 20.565 |
| pCVQZ       | 348.828 | 30.593 | 37.859 | 20.891 | 349.004 | 30.632 | 37.787 | 20.910 |
| pCV5Z       | 346.235 | 30.420 | 42.949 | 21.018 | 346.338 | 30.437 | 42.931 | 21.030 |
| pCV6Z       | 345.746 | 30.375 | 44.734 | 21.053 | 345.759 | 30.378 | 44.724 | 21.055 |
| aug-pCVDZ   | 352.625 | 31.253 | 41.599 | 19.819 | 349.123 | 30.974 | 41.338 | 19.391 |
| aug-pCVTZ   | 346.222 | 30.765 | 44.727 | 20.597 | 345.012 | 30.656 | 44.624 | 20.440 |
| aug-pCVQZ   | 345.915 | 30.488 | 45.414 | 20.913 | 345.613 | 30.465 | 45.382 | 20.872 |
| aug-pCV5Z   | 345.730 | 30.400 | 45.696 | 21.027 | 345.647 | 30.394 | 45.685 | 21.015 |
| aug-pCV6Z   | 345.713 | 30.362 | 45.773 | 21.075 | 345.640 | 30.356 | 45.766 | 21.065 |
| aug-pc-1    | 353.674 | 31.104 | 40.141 | 20.078 | 350.035 | 30.784 | 39.897 | 19.612 |
| aug-pc-2    | 344.536 | 30.741 | 45.430 | 20.710 | 343.916 | 30.689 | 45.383 | 20.630 |
| aug-pc-3    | 345.415 | 30.465 | 45.863 | 21.001 | 345.052 | 30.443 | 45.806 | 20.951 |
| aug-pc-4    | 345.952 | 30.407 | 45.397 | 21.067 | 345.574 | 30.382 | 45.343 | 21.014 |
| aug-pc5-1   | 345.057 | 30.642 | 47.150 | 20.521 | 341.350 | 30.309 | 46.924 | 20.034 |
| aug-pc5-2   | 346.959 | 30.610 | 46.150 | 20.857 | 346.318 | 30.551 | 46.117 | 20.773 |
| aug-pc5-3   | 345.759 | 30.439 | 45.537 | 21.028 | 345.369 | 30.416 | 45.476 | 20.973 |
| aug-pc5-4   | 345.942 | 30.404 | 45.394 | 21.070 | 345.572 | 30.379 | 45.341 | 21.018 |
| Basis sets | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|----------------------------|---------------------------|
|            | Shielding          | Anisotropy | Shielding          | Anisotropy |
|            | O | H | O | H | O | H | O | H |
| pVDZ       | 355.258 | 31.824 | 24.087 | 19.132 | 351.657 | 31.678 | 23.881 | 18.722 |
| pVTZ       | 343.824 | 31.214 | 35.463 | 20.202 | 343.946 | 31.261 | 35.308 | 20.210 |
| pVQZ       | 340.343 | 30.840 | 44.248 | 20.507 | 341.259 | 30.926 | 44.200 | 20.613 |
| pV5Z       | 337.881 | 30.686 | 48.408 | 20.622 | 338.769 | 30.756 | 48.411 | 20.727 |
| pV6Z       | 337.237 | 30.646 | 50.152 | 20.655 | 338.088 | 30.709 | 50.154 | 20.755 |
| aug-pVDZ   | 346.104 | 31.527 | 45.502 | 19.399 | 342.860 | 31.271 | 45.509 | 19.011 |
| aug-pVTZ   | 337.932 | 31.044 | 49.534 | 20.193 | 337.203 | 30.984 | 49.531 | 20.109 |
| aug-pVQZ   | 337.736 | 30.756 | 50.366 | 20.522 | 338.231 | 30.793 | 50.365 | 20.581 |
| aug-pV5Z   | 337.170 | 30.673 | 50.840 | 20.627 | 337.917 | 30.727 | 50.840 | 20.716 |
| aug-pV6Z   | 337.146 | 30.637 | 50.909 | 20.670 | 337.931 | 30.694 | 50.912 | 20.764 |
| pCVTZ      | 343.852 | 31.175 | 36.919 | 20.205 | 344.489 | 31.259 | 36.799 | 20.273 |
| pCVQZ      | 339.779 | 30.806 | 44.380 | 20.505 | 341.090 | 30.919 | 44.343 | 20.657 |
| pCV5Z      | 337.332 | 30.652 | 48.958 | 20.625 | 338.676 | 30.753 | 48.962 | 20.784 |
| pCV6Z      | 336.891 | 30.611 | 50.464 | 20.659 | 338.193 | 30.706 | 50.470 | 20.813 |
| aug-pCVTZ  | 344.373 | 31.513 | 46.533 | 19.409 | 341.439 | 31.282 | 46.529 | 19.057 |
| aug-pCVQZ  | 337.633 | 31.007 | 50.086 | 20.196 | 337.403 | 30.985 | 50.098 | 20.170 |
| aug-pCV5Z  | 337.203 | 30.723 | 50.890 | 20.521 | 338.117 | 30.789 | 50.894 | 20.629 |
| aug-pCV6Z  | 336.917 | 30.638 | 51.206 | 20.630 | 338.114 | 30.724 | 51.208 | 20.772 |
| aug-pc-1   | 345.138 | 31.368 | 45.036 | 19.638 | 341.713 | 31.105 | 45.056 | 19.252 |
| aug-pc-2   | 335.877 | 30.987 | 50.737 | 20.305 | 336.232 | 31.010 | 50.747 | 20.346 |
| aug-pc-3   | 336.638 | 30.695 | 51.310 | 20.611 | 337.398 | 30.754 | 51.300 | 20.700 |
| aug-pc-4   | 337.115 | 30.642 | 50.909 | 20.670 | 337.915 | 30.703 | 50.902 | 20.765 |
| aug-pcS1   | 336.207 | 30.902 | 52.022 | 20.087 | 332.731 | 30.626 | 52.075 | 19.682 |
| aug-pcS2   | 338.346 | 30.854 | 51.430 | 20.455 | 338.636 | 30.867 | 51.451 | 20.491 |
| aug-pcS3   | 336.998 | 30.670 | 50.993 | 20.637 | 337.730 | 30.728 | 50.982 | 20.723 |
| aug-pcS4   | 337.100 | 30.639 | 50.911 | 20.674 | 337.910 | 30.701 | 50.904 | 20.770 |
### Table S: CCSD(T): shieldings and shielding anisotropies

| Basis sets | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|------------------------------|---------------------------|
|            | Shielding | Anisotropy | Shielding | Anisotropy |
|            | O  | H  | O  | H  | O  | H  | O  | H  |
| pVDZ       | 355.139 | 31.876 | 23.325 | 19.047 | 350.802 | 31.697 | 22.997 | 18.555 |
| pVTZ       | 344.597 | 31.250 | 34.143 | 20.149 | 343.671 | 31.224 | 33.893 | 20.034 |
| pVQZ       | 341.310 | 30.864 | 42.874 | 20.468 | 341.036 | 30.865 | 42.786 | 20.433 |
| pV5Z       | 338.867 | 30.703 | 47.099 | 20.590 | 338.495 | 30.680 | 47.067 | 20.544 |
| pV6Z       | 338.201 | 30.660 | 48.914 | 20.623 | 337.757 | 30.628 | 48.900 | 20.570 |
| aug-pVDZ   | 346.433 | 31.555 | 44.723 | 19.351 | 342.243 | 31.235 | 44.658 | 18.848 |
| aug-pVTZ   | 338.787 | 31.061 | 48.407 | 20.159 | 336.819 | 30.905 | 48.340 | 19.930 |
| aug-pVQZ   | 338.652 | 30.770 | 49.201 | 20.491 | 337.871 | 30.711 | 49.185 | 20.398 |
| aug-pV5Z   | 338.108 | 30.686 | 49.659 | 20.596 | 337.555 | 30.644 | 49.651 | 20.530 |
| aug-pV6Z   | 338.095 | 30.650 | 49.723 | 20.640 | 337.572 | 30.610 | 49.719 | 20.577 |
| pCVTZ      | 353.893 | 31.865 | 23.559 | 19.057 | 349.979 | 31.711 | 23.165 | 18.605 |
| pCVQZ      | 344.681 | 31.210 | 35.581 | 20.150 | 344.206 | 31.217 | 35.388 | 20.089 |
| pCV5Z      | 340.776 | 30.831 | 42.974 | 20.465 | 340.850 | 30.855 | 42.907 | 20.471 |
| pCV6Z      | 338.339 | 30.669 | 47.636 | 20.592 | 338.379 | 30.674 | 47.629 | 20.596 |
| pCVDZ      | 353.893 | 31.865 | 23.559 | 19.057 | 349.979 | 31.711 | 23.165 | 18.605 |
| aug-pCVDZ  | 344.735 | 31.542 | 45.756 | 19.360 | 340.834 | 31.244 | 45.680 | 18.890 |
| aug-pCVTZ  | 338.538 | 31.024 | 48.930 | 20.161 | 337.005 | 30.901 | 48.903 | 19.985 |
| aug-pCVQZ  | 338.153 | 30.737 | 49.702 | 20.489 | 337.741 | 30.703 | 49.703 | 20.440 |
| aug-pCV5Z  | 338.886 | 30.652 | 50.006 | 20.598 | 337.744 | 30.638 | 50.015 | 20.582 |
| aug-pCV6Z  | 337.827 | 30.616 | 50.094 | 20.643 | 337.720 | 30.604 | 50.105 | 20.631 |
| aug-pC-1   | 345.391 | 31.396 | 44.375 | 19.588 | 341.123 | 31.078 | 44.332 | 19.106 |
| aug-pC-2   | 336.616 | 31.007 | 49.644 | 20.265 | 335.773 | 30.944 | 49.635 | 20.168 |
| aug-pC-3   | 337.561 | 30.710 | 50.151 | 20.577 | 337.046 | 30.676 | 50.127 | 20.515 |
| aug-pC-4   | 338.052 | 30.655 | 49.728 | 20.639 | 337.556 | 30.621 | 49.711 | 20.579 |
| aug-pC-5-1 | 336.872 | 30.923 | 51.065 | 20.045 | 332.351 | 30.577 | 51.017 | 19.516 |
| aug-pC-5-2 | 339.141 | 30.872 | 50.298 | 20.415 | 338.244 | 30.799 | 50.305 | 20.311 |
| aug-pC-5-3 | 337.914 | 30.685 | 49.831 | 20.603 | 337.371 | 30.649 | 49.804 | 20.537 |
| aug-pC-5-4 | 338.038 | 30.653 | 49.729 | 20.642 | 337.552 | 30.619 | 49.713 | 20.583 |
### Tabel 56: HF: vibrational corrections to shieldings and shielding anisotropies

| Basis sets | Relative to the Experimental Geometry (ExpC) | Relative to the Optimized Geometry (ZPVC) |
|------------|---------------------------------------------|------------------------------------------|
|            | Shielding        | Anisotropy       | Shielding        | Anisotropy       |
|            | O    | H    | O    | H       | O    | H       | O    | H       |
| pVDZ       | -5.712 | -0.073 | -1.693 | -0.337 | -11.502 | -0.509 | -1.268 | -0.939 |
| pVTZ       | -2.092 | 0.097  | -1.569 | -0.056 | -10.156 | -0.525 | -1.099 | -0.929 |
| pVQZ       | -1.665 | 0.113  | -1.578 | 0.014  | -10.323 | -0.519 | -0.981 | -0.928 |
| pV5Z       | -1.605 | 0.106  | -1.507 | 0.021  | -10.330 | -0.517 | -0.937 | -0.928 |
| pV6Z       | -1.634 | 0.103  | -1.561 | 0.022  | -10.415 | -0.517 | -0.903 | -0.927 |
| aug-pVDZ   | -3.823 | -0.050 | -1.315 | -0.172 | -10.478 | -0.524 | -0.761 | -0.893 |
| aug-pVTZ   | -2.231 | 0.056  | -1.485 | -0.068 | -10.128 | -0.528 | -1.004 | -0.906 |
| aug-pVQZ   | -1.717 | 0.098  | -1.574 | 0.004  | -10.320 | -0.519 | -0.904 | -0.925 |
| aug-pV5Z   | -1.660 | 0.103  | -1.587 | 0.016  | -10.414 | -0.517 | -0.902 | -0.928 |
| aug-pV6Z   | -1.630 | 0.100  | -1.590 | 0.020  | -10.410 | -0.520 | -0.906 | -0.929 |
| aug-pc-1   | -4.349 | -0.078 | -1.508 | -0.234 | -10.935 | -0.521 | -1.000 | -0.899 |
| aug-pc-2   | -1.538 | 0.109  | -1.469 | 0.005  | -10.574 | -0.523 | -0.796 | -0.932 |
| aug-pc-3   | -1.587 | 0.104  | -1.640 | 0.023  | -10.425 | -0.517 | -0.953 | -0.926 |
| aug-pc-4   | -1.549 | 0.101  | -1.586 | 0.021  | -10.320 | -0.518 | -0.901 | -0.928 |
| aug-pcS-1  | -4.196 | -0.086 | -1.396 | -0.233 | -10.576 | -0.502 | -1.213 | -0.923 |
| aug-pcS-2  | -1.551 | 0.109  | -1.670 | 0.021  | -10.399 | -0.511 | -0.965 | -0.931 |
| aug-pcS-3  | -1.618 | 0.101  | -1.594 | 0.021  | -10.387 | -0.517 | -0.905 | -0.929 |
| aug-pcS-4  | -1.606 | 0.102  | -1.587 | 0.022  | -10.385 | -0.517 | -0.901 | -0.929 |

### Tabel 57: B3LYP: vibrational corrections to shieldings and shielding anisotropies

| Basis sets | Relative to the Experimental Geometry (ExpC) | Relative to the Optimized Geometry (ZPVC) |
|------------|---------------------------------------------|------------------------------------------|
|            | Shielding        | Anisotropy       | Shielding        | Anisotropy       |
|            | O    | H    | O    | H       | O    | H       | O    | H       |
| pVDZ       | -22.954 | -0.827 | -3.734 | -1.813 | -16.053 | -0.517 | -3.833 | -1.139 |
| pVTZ       | -15.865 | -0.688 | -2.545 | -1.319 | -13.545 | -0.522 | -2.590 | -1.083 |
| pVQZ       | -15.105 | -0.657 | -2.267 | -1.239 | -13.385 | -0.514 | -2.401 | -1.063 |
| pV5Z       | -14.836 | -0.667 | -2.119 | -1.223 | -13.103 | -0.510 | -2.313 | -1.048 |
| pV6Z       | -14.804 | -0.671 | -2.092 | -1.222 | -13.033 | -0.510 | -2.306 | -1.045 |
| aug-pVDZ   | -17.035 | -0.828 | -1.924 | -1.435 | -12.960 | -0.521 | -2.039 | -1.004 |
| aug-pVTZ   | -15.282 | -0.745 | -2.069 | -1.281 | -12.736 | -0.521 | -2.279 | -1.026 |
| aug-pVQZ   | -14.918 | -0.687 | -1.970 | -1.230 | -13.009 | -0.515 | -2.188 | -1.038 |
| aug-pV5Z   | -14.915 | -0.677 | -1.994 | -1.225 | -13.088 | -0.512 | -2.217 | -1.043 |
| aug-pV6Z   | -14.955 | -0.675 | -2.046 | -1.226 | -13.151 | -0.511 | -2.268 | -1.045 |
| aug-pc-1   | -18.347 | -0.875 | -2.206 | -1.509 | -13.426 | -0.515 | -2.365 | -1.015 |
| aug-pc-2   | -15.246 | -0.700 | -1.818 | -1.248 | -13.157 | -0.516 | -2.071 | -1.043 |
| aug-pc-3   | -14.965 | -0.676 | -1.993 | -1.226 | -13.148 | -0.511 | -2.219 | -1.045 |
| aug-pc-4   | -14.699 | -0.676 | -2.657 | -1.223 | -12.892 | -0.513 | -2.882 | -1.043 |
| aug-pcS-1  | -17.800 | -0.823 | -2.264 | -1.498 | -13.425 | -0.502 | -2.547 | -1.040 |
| aug-pcS-2  | -14.937 | -0.677 | -2.025 | -1.224 | -13.092 | -0.506 | -2.259 | -1.042 |
| aug-pcS-3  | -14.952 | -0.674 | -1.992 | -1.226 | -13.146 | -0.511 | -2.213 | -1.046 |
| aug-pcS-4  | -14.935 | -0.671 | -2.048 | -1.231 | -13.138 | -0.508 | -2.270 | -1.051 |
Tabel S8: MP2: vibrational corrections to shieldings and shielding anisotropies

| Basis sets | Relative to the Experimental Geometry (ExpC) | Relative to the Optimized Geometry (ZPVC) |
|------------|---------------------------------------------|------------------------------------------|
|            | Shielding | Anisotropy | Shielding | Anisotropy |
|            | O   | H   | O   | H   | O   | H   | O   | H   |
| pVDZ       | -14.615 | -0.628 | -3.811 | -1.434 | -11.492 | -0.501 | -3.451 | -1.034 |
| pVTZ       | -10.134 | -0.525 | -3.440 | -1.078 | -9.506  | -0.517 | -3.162 | -0.985 |
| pVQZ       | -9.378  | -0.499 | -3.007 | -0.999 | -9.242  | -0.514 | -2.898 | -0.976 |
| pV5Z       | -9.275  | -0.526 | -2.832 | -1.005 | -9.099  | -0.513 | -2.769 | -0.966 |
| pV6Z       | -9.364  | -0.539 | -2.758 | -1.010 | -9.004  | -0.514 | -2.708 | -0.960 |
| aug-pVDZ   | -12.598 | -0.826 | -2.890 | -1.395 | -9.236  | -0.524 | -2.636 | -0.938 |
| aug-pVTZ   | -10.491 | -0.666 | -3.015 | -1.148 | -8.882  | -0.521 | -2.850 | -0.938 |
| aug-pVQZ   | -9.604  | -0.567 | -2.753 | -1.044 | -8.970  | -0.517 | -2.686 | -0.958 |
| aug-pV5Z   | -9.425  | -0.550 | -2.730 | -1.024 | -8.974  | -0.516 | -2.683 | -0.963 |
| aug-pV6Z   | -9.406  | -0.550 | -2.713 | -1.022 | -8.958  | -0.514 | -2.671 | -0.961 |
| pCVDZ      | -14.205 | -0.606 | -3.990 | -1.399 | -11.427 | -0.502 | -3.570 | -1.033 |
| pCVTZ      | -9.851  | -0.487 | -3.297 | -1.021 | -9.652  | -0.517 | -3.101 | -0.984 |
| pCVQZ      | -9.047  | -0.475 | -2.914 | -0.956 | -9.223  | -0.514 | -2.842 | -0.975 |
| pCV5Z      | -8.922  | -0.496 | -2.718 | -0.953 | -9.024  | -0.513 | -2.700 | -0.965 |
| pCV6Z      | ---     | ---    | ---    | ---    | ---     | ---    | ---    | ---    |
| aug-pCVDZ  | -12.369 | -0.804 | -3.014 | -1.369 | -9.227  | -0.525 | -2.753 | -0.941 |
| aug-pCVTZ  | -10.224 | -0.631 | -2.867 | -1.097 | -9.013  | -0.522 | -2.764 | -0.940 |
| aug-pCVQZ  | -9.299  | -0.540 | -2.677 | -0.999 | -8.997  | -0.517 | -2.645 | -0.958 |
| aug-pCV5Z  | -9.067  | -0.521 | -2.615 | -0.973 | -8.984  | -0.515 | -2.604 | -0.961 |
| aug-pCV6Z  | -9.046  | -0.521 | -2.602 | -0.972 | -8.972  | -0.515 | -2.595 | -0.962 |
| aug-pc-1   | -12.977 | -0.836 | -3.178 | -1.407 | -9.337  | -0.517 | -2.934 | -0.941 |
| aug-pc-2   | -9.745  | -0.572 | -2.643 | -1.041 | -9.125  | -0.519 | -2.596 | -0.961 |
| aug-pc-3   | -9.434  | -0.536 | -2.818 | -1.013 | -9.071  | -0.514 | -2.761 | -0.963 |
| aug-pc-4   | -9.377  | -0.539 | -2.734 | -1.018 | -8.999  | -0.514 | -2.680 | -0.965 |
| aug-pcS-1  | -13.030 | -0.826 | -3.364 | -1.448 | -9.324  | -0.494 | -3.138 | -0.961 |
| aug-pcS-2  | -9.677  | -0.563 | -2.793 | -1.043 | -9.036  | -0.504 | -2.760 | -0.959 |
| aug-pcS-3  | -9.439  | -0.537 | -2.798 | -1.020 | -9.049  | -0.513 | -2.737 | -0.965 |
| aug-pcS-4  | -9.370  | -0.538 | -2.732 | -1.017 | -9.000  | -0.514 | -2.679 | -0.965 |
| Basis sets | Relative to the Experimental Geometry (ExpC) | Relative to the Optimized Geometry (ZPVC) |
|-----------|--------------------------------------------|----------------------------------------|
|           | Shielding          | Anisotropy      | Shielding          | Anisotropy      |
|           | O   | H   | O   | H   | O   | H   | O   | H   |
| pVDZ      |   -16.656 | -0.651 | -3.098 | -1.481 |   -13.056 | -0.505 | -2.892 | -1.071 |
| pVTZ      |   -10.953 | -0.470 | -2.553 | -1.016 |   -11.074 | -0.517 | -2.398 | -1.024 |
| pVQZ      |   -9.988  | -0.425 | -2.137 | -0.911 |   -10.904 | -0.510 | -2.089 | -1.017 |
| pV5Z      |   -9.869  | -0.438 | -1.964 | -0.904 |   -10.757 | -0.508 | -1.967 | -1.009 |
| pV6Z      |   -9.921  | -0.445 | -1.919 | -0.906 |   -10.772 | -0.508 | -1.921 | -1.006 |
| aug-pVDZ  |   -14.315 | -0.776 | -1.949 | -1.371 |   -11.071 | -0.520 | -1.956 | -0.983 |
| aug-pVTZ  |   -11.375 | -0.576 | -2.111 | -1.068 |   -10.646 | -0.517 | -2.108 | -0.984 |
| aug-pVQZ  |   -10.225 | -0.475 | -1.919 | -0.943 |   -10.720 | -0.512 | -1.918 | -1.002 |
| aug-pV5Z  |   -9.994  | -0.455 | -1.909 | -0.918 |   -10.741 | -0.509 | -1.909 | -1.007 |
| aug-pV6Z  |   -9.905  | -0.448 | -1.891 | -0.908 |   -10.690 | -0.505 | -1.894 | -1.002 |
| pCVDZ     |   -16.149 | -0.625 | -3.250 | -1.437 |   -12.980 | -0.506 | -2.983 | -1.069 |
| pCVTZ     |   -10.579 | -0.432 | -2.455 | -0.956 |   -11.215 | -0.517 | -2.355 | -1.024 |
| pCVQZ     |   -9.555  | -0.397 | -2.071 | -0.863 |   -10.866 | -0.510 | -2.034 | -1.015 |
| pCV5Z     |   -9.399  | -0.407 | -1.900 | -0.849 |   -10.743 | -0.508 | -1.904 | -1.008 |
| pCV6Z     |   ---     | ---     | ---     | ---     |   ---     | ---     | ---     | ---     |
| aug-pCVDZ |   -13.991 | -0.752 | -2.049 | -1.337 |   -11.058 | -0.521 | -2.045 | -0.985 |
| aug-pCVTZ |   -10.995 | -0.539 | -2.008 | -1.010 |   -10.765 | -0.517 | -2.020 | -0.984 |
| aug-pCVQZ |   -9.813  | -0.446 | -1.874 | -0.893 |   -10.727 | -0.511 | -1.878 | -1.001 |
| aug-pCV5Z |   -9.528  | -0.423 | -1.835 | -0.863 |   -10.725 | -0.509 | -1.837 | -1.005 |
| aug-pCV6Z |   ---     | ---     | ---     | ---     |   ---     | ---     | ---     | ---     |
| aug-pc-1  |   -14.706 | -0.776 | -2.235 | -1.370 |   -11.280 | -0.513 | -2.255 | -0.984 |
| aug-pc-2  |   -10.591 | -0.493 | -1.883 | -0.968 |   -10.946 | -0.516 | -1.893 | -1.009 |
| aug-pc-3  |   -10.100 | -0.449 | -1.999 | -0.922 |   -10.860 | -0.508 | -1.989 | -1.011 |
| aug-pc-4  |   -9.972  | -0.444 | -1.948 | -0.915 |   -10.772 | -0.505 | -1.941 | -1.010 |
| aug-pc5-1 |   -14.722 | -0.767 | -2.428 | -1.412 |   -11.246 | -0.491 | -2.481 | -1.007 |
| aug-pc5-2 |   -10.538 | -0.487 | -2.037 | -0.971 |   -10.828 | -0.500 | -2.058 | -1.007 |
| aug-pc5-3 |   -10.092 | -0.449 | -1.953 | -0.926 |   -10.824 | -0.506 | -1.942 | -1.012 |
| aug-pc5-4 |   -10.009 | -0.447 | -1.981 | -0.921 |   -10.819 | -0.509 | -1.974 | -1.017 |
### Tabel S10: CCSD(T): vibrational corrections to shieldings and shielding anisotropies

| Basis sets | Relative to the Experimental Geometry (ExpC) | Relative to the Optimized Geometry (ZPVC) |
|------------|---------------------------------------------|------------------------------------------|
|            | Shielding | Anisotropy | Shielding | Anisotropy |
|            | O | H | O | H | O | H | O | H |
| pVDZ       | -17.877 | -0.665 | -3.502 | -1.591 | -13.541 | -0.506 | -3.174 | -1.099 |
| pVTZ       | -12.342 | -0.543 | -2.952 | -1.165 | -11.398 | -0.517 | -2.702 | -1.050 |
| pVQZ       | -11.440 | -0.510 | -2.473 | -1.076 | -11.165 | -0.511 | -2.385 | -1.041 |
| pV5Z       | -11.362 | -0.532 | -2.285 | -1.077 | -10.990 | -0.508 | -2.253 | -1.031 |
| pV6Z       | -11.444 | -0.542 | -2.219 | -1.081 | -11.000 | -0.510 | -2.205 | -1.028 |
| aug-pVDZ   | -15.554 | -0.843 | -2.244 | -1.509 | -11.364 | -0.522 | -2.179 | -1.006 |
| aug-pVTZ   | -12.837 | -0.673 | -2.448 | -1.234 | -10.869 | -0.517 | -2.381 | -1.005 |
| aug-pVQZ   | -11.723 | -0.572 | -2.209 | -1.117 | -10.942 | -0.513 | -2.193 | -1.024 |
| aug-pV5Z   | -11.519 | -0.553 | -2.195 | -1.094 | -10.966 | -0.511 | -2.187 | -1.028 |
| aug-pV6Z   | -11.494 | -0.549 | -2.170 | -1.092 | -10.971 | -0.509 | -2.166 | -1.029 |
| pCVDZ      | -17.386 | -0.661 | -3.663 | -1.550 | -13.471 | -0.507 | -3.269 | -1.098 |
| pCVTZ      | -12.023 | -0.509 | -2.843 | -1.111 | -11.548 | -0.516 | -2.650 | -1.050 |
| pCVQZ      | -11.060 | -0.487 | -2.402 | -1.033 | -11.134 | -0.511 | -2.335 | -1.039 |
| pCV5Z      | -10.937 | -0.504 | -2.203 | -1.026 | -10.977 | -0.509 | -2.196 | -1.030 |
| pCV6Z      | ---     | ---     | ---     | ---     | ---     | ---     | ---     | ---     |
| aug-pCVDZ  | -15.254 | -0.821 | -2.351 | -1.477 | -11.353 | -0.523 | -2.275 | -1.007 |
| aug-pCVTZ  | -12.527 | -0.640 | -2.330 | -1.183 | -10.994 | -0.518 | -2.303 | -1.007 |
| aug-pCVQZ  | -11.365 | -0.546 | -2.158 | -1.072 | -10.953 | -0.513 | -2.159 | -1.023 |
| aug-pCV5Z  | -11.095 | -0.525 | -2.110 | -1.044 | -10.952 | -0.511 | -2.119 | -1.028 |
| aug-pCV6Z  | -11.088 | -0.525 | -2.082 | -1.044 | -10.981 | -0.514 | -2.093 | -1.032 |
| aug-pc-1   | -15.861 | -0.832 | -2.515 | -1.488 | -11.593 | -0.515 | -2.472 | -1.006 |
| aug-pc-2   | -12.029 | -0.580 | -2.180 | -1.127 | -11.186 | -0.517 | -2.171 | -1.030 |
| aug-pc-3   | -11.591 | -0.542 | -2.331 | -1.094 | -11.076 | -0.508 | -2.307 | -1.032 |
| aug-pc-4   | -11.418 | -0.535 | -2.159 | -1.086 | -10.922 | -0.501 | -2.142 | -1.026 |
| aug-pcS-1  | -16.019 | -0.838 | -2.784 | -1.558 | -11.498 | -0.492 | -2.736 | -1.029 |
| aug-pcS-2  | -11.951 | -0.574 | -2.324 | -1.131 | -11.054 | -0.501 | -2.331 | -1.027 |
| aug-pcS-3  | -11.611 | -0.543 | -2.275 | -1.101 | -11.068 | -0.507 | -2.248 | -1.035 |
| aug-pcS-4  | -11.452 | -0.541 | -2.214 | -1.090 | -10.966 | -0.507 | -2.198 | -1.031 |
Tabel S11: HF: extrapolated shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Used cardinal numbers | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|----------------------|-------------------------------|----------------------------|
|            |                      | Shielding | Anisotropy | Shielding | Anisotropy |
|            |                      | O   | H   | O   | H   | O   | H   |
| cc-pVXZ    | D-T                  | 330.433 | 30.607 | 47.385 | 21.121 | 339.455 | 31.306 | 46.896 | 22.107 |
|            | T-Q                  | 328.450 | 30.444 | 57.414 | 20.959 | 337.542 | 31.083 | 56.726 | 21.951 |
|            | Q-5                  | 325.653 | 30.397 | 59.483 | 20.988 | 334.448 | 31.009 | 58.940 | 21.944 |
|            | 5-6                  | 327.025 | 30.447 | 58.828 | 20.965 | 335.884 | 31.065 | 58.047 | 21.916 |
| aug-cc-pVXZ| D-T                 | 325.241 | 30.563 | 58.270 | 20.933 | 333.661 | 31.193 | 57.820 | 21.820 |
|            | T-Q                  | 328.412 | 30.427 | 57.271 | 20.990 | 337.530 | 31.069 | 56.463 | 21.986 |
|            | Q-5                  | 327.207 | 30.443 | 57.739 | 20.999 | 336.120 | 31.066 | 57.038 | 21.959 |
|            | 5-6                  | 327.763 | 30.443 | 57.423 | 20.994 | 336.560 | 31.062 | 56.740 | 21.949 |
| aug-pc-n   | 1-2                  | 322.402 | 30.523 | 59.765 | 20.994 | 332.470 | 31.234 | 59.023 | 22.046 |
|            | 2-3                  | 328.307 | 30.362 | 57.855 | 21.097 | 337.000 | 30.974 | 57.156 | 22.056 |
|            | 3-4                  | 328.321 | 30.444 | 56.973 | 20.995 | 337.023 | 31.061 | 56.290 | 21.945 |
| aug-pcS-n  | 1-2                  | 330.658 | 30.571 | 57.473 | 20.982 | 340.546 | 31.278 | 56.548 | 22.044 |
|            | 2-3                  | 326.802 | 30.400 | 57.084 | 21.050 | 335.513 | 31.017 | 56.406 | 21.998 |
|            | 3-4                  | 327.844 | 30.464 | 57.287 | 20.968 | 336.633 | 31.084 | 56.604 | 21.919 |

Tabel S12: B3LYP: extrapolated shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Used cardinal numbers | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|----------------------|-------------------------------|----------------------------|
|            |                      | Shielding | Anisotropy | Shielding | Anisotropy |
|            |                      | O   | H   | O   | H   | O   | H   |
| cc-pVXZ    | D-T                  | 332.138 | 31.297 | 39.744 | 19.945 | 331.745 | 31.192 | 39.955 | 19.894 |
|            | T-Q                  | 328.219 | 31.026 | 53.735 | 19.792 | 326.938 | 30.900 | 53.934 | 19.660 |
|            | Q-5                  | 324.576 | 30.909 | 57.641 | 19.851 | 322.830 | 30.737 | 57.898 | 19.677 |
|            | 5-6                  | 325.337 | 30.998 | 57.813 | 19.766 | 323.514 | 30.833 | 58.055 | 19.586 |
| aug-cc-pVXZ| D-T                 | 324.949 | 31.161 | 55.568 | 19.765 | 323.046 | 30.972 | 55.819 | 19.584 |
|            | T-Q                  | 327.491 | 30.989 | 55.560 | 19.805 | 326.048 | 30.855 | 55.782 | 19.659 |
|            | Q-5                  | 326.030 | 30.991 | 56.181 | 19.829 | 324.290 | 30.833 | 56.409 | 19.657 |
|            | 5-6                  | 326.565 | 30.997 | 55.822 | 19.815 | 324.792 | 30.837 | 56.042 | 19.637 |
| aug-pc-n   | 1-2                  | 322.723 | 31.115 | 57.582 | 19.771 | 321.826 | 31.006 | 57.874 | 19.688 |
|            | 2-3                  | 326.773 | 30.919 | 55.988 | 19.937 | 325.155 | 30.769 | 56.194 | 19.773 |
|            | 3-4                  | 326.860 | 30.996 | 55.668 | 19.821 | 325.064 | 30.834 | 55.892 | 19.641 |
| aug-pcS-n  | 1-2                  | 329.455 | 31.123 | 55.671 | 19.798 | 328.675 | 31.015 | 55.884 | 19.729 |
|            | 2-3                  | 325.524 | 30.961 | 55.361 | 19.876 | 323.745 | 30.803 | 55.573 | 19.697 |
|            | 3-4                  | 326.759 | 31.014 | 55.647 | 19.794 | 324.971 | 30.852 | 55.869 | 19.616 |
Table S13: MP2: extrapolated shieldings using the inverse-third-power functions and specified basis sets

| Basis sets       | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------------|------------------------------|---------------------------|
|                  | Shielding                   | Anisotropy                | Shielding                   | Anisotropy |
| Series           | Used cardinal numbers       | O  | H  | O  | H  | O  | H  | O  | H  |
| cc-pVXZ D-T      | 348.358                     | 30.749 | 33.147 | 21.053 | 348.781 | 30.792 | 32.904 | 21.089 |
| T-Q              | 346.946                     | 30.355 | 44.395 | 21.111 | 347.169 | 30.387 | 44.409 | 21.139 |
| Q-5              | 344.217                     | 30.276 | 47.145 | 21.146 | 343.812 | 30.233 | 47.131 | 21.090 |
| 5-6              | 345.140                     | 30.347 | 47.265 | 21.096 | 344.654 | 30.305 | 47.233 | 21.031 |
| aug-cc-pVXZ D-T  | 343.348                     | 30.607 | 45.647 | 20.925 | 342.477 | 30.528 | 45.520 | 20.819 |
| T-Q              | 346.450                     | 30.319 | 45.381 | 21.150 | 346.528 | 30.338 | 45.385 | 21.155 |
| Q-5              | 345.564                     | 30.343 | 45.765 | 21.141 | 345.305 | 30.323 | 45.739 | 21.107 |
| 5-6              | 346.098                     | 30.345 | 45.433 | 21.138 | 345.654 | 30.307 | 45.398 | 21.077 |
| cc-pCVXZ D-T     | 348.964                     | 30.694 | 35.327 | 21.050 | 349.851 | 30.780 | 35.225 | 21.151 |
| T-Q              | 345.892                     | 30.325 | 43.444 | 21.102 | 346.341 | 30.371 | 43.463 | 21.162 |
| Q-5              | 343.514                     | 30.238 | 48.289 | 21.151 | 343.541 | 30.232 | 48.328 | 21.156 |
| 5-6              | 345.074                     | 30.313 | 47.186 | 21.101 | 344.964 | 30.297 | 47.187 | 21.089 |
| aug-cc-pCVXZ D-T | 343.678                     | 30.560 | 46.044 | 20.925 | 343.281 | 30.522 | 46.008 | 20.882 |
| T-Q              | 345.691                     | 30.286 | 45.915 | 21.144 | 346.052 | 30.326 | 45.935 | 21.187 |
| Q-5              | 345.536                     | 30.308 | 45.992 | 21.147 | 345.683 | 30.320 | 46.003 | 21.165 |
| 5-6              | 345.690                     | 30.310 | 45.879 | 21.141 | 345.630 | 30.304 | 45.877 | 21.134 |
| aug-pc-n 1-2     | 340.688                     | 30.588 | 47.657 | 20.976 | 341.340 | 30.649 | 47.693 | 21.059 |
| 2-3              | 346.056                     | 30.264 | 46.179 | 21.213 | 345.881 | 30.263 | 46.115 | 21.185 |
| 3-4              | 346.515                     | 30.346 | 44.908 | 21.136 | 346.122 | 30.318 | 44.857 | 21.080 |
| aug-pcS-n 1-2    | 347.760                     | 30.597 | 45.729 | 20.998 | 348.410 | 30.653 | 45.777 | 21.084 |
| 2-3              | 344.883                     | 30.314 | 45.090 | 21.153 | 344.676 | 30.317 | 45.008 | 21.119 |
| 3-4              | 346.134                     | 30.367 | 45.244 | 21.114 | 345.785 | 30.340 | 45.199 | 21.065 |
### Table S14: CCSD: extrapolated shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Series | Used cardinal numbers | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|------------|--------|------------------------|------------------------------|----------------------------|
|            |        |                        | Shielding | Anisotropy | Shielding | Anisotropy |
|            |        |                        | O | H | O | H | O | H | O | H |
| cc-pVXZ    | D-T    |                        | 339.010 | 30.957 | 40.253 | 20.653 | 340.699 | 31.085 | 40.119 | 20.837 |
|            | T-Q    |                        | 337.803 | 30.567 | 50.659 | 20.730 | 339.298 | 30.682 | 50.689 | 20.907 |
|            | Q-5    |                        | 335.298 | 30.524 | 52.773 | 20.743 | 336.157 | 30.578 | 52.829 | 20.847 |
|            | 5-6    |                        | 336.352 | 30.591 | 52.548 | 20.700 | 337.153 | 30.644 | 52.548 | 20.793 |
| aug-cc-pVXZ| D-T    |                        | 334.491 | 30.841 | 51.232 | 20.527 | 334.821 | 30.863 | 51.224 | 20.571 |
|            | T-Q    |                        | 337.593 | 30.546 | 50.973 | 20.762 | 338.981 | 30.654 | 50.974 | 20.925 |
|            | Q-5    |                        | 336.576 | 30.586 | 51.337 | 20.737 | 337.588 | 30.658 | 51.338 | 20.858 |
|            | 5-6    |                        | 337.113 | 30.588 | 51.004 | 20.729 | 337.950 | 30.649 | 51.011 | 20.830 |
| cc-pCVXZ   | D-T    |                        | 339.579 | 30.907 | 42.217 | 20.652 | 341.819 | 31.076 | 42.159 | 20.904 |
|            | T-Q    |                        | 336.807 | 30.537 | 49.825 | 20.724 | 338.610 | 30.671 | 49.848 | 20.937 |
|            | Q-5    |                        | 334.765 | 30.490 | 53.761 | 20.751 | 336.143 | 30.579 | 53.808 | 20.917 |
|            | 5-6    |                        | 336.285 | 30.555 | 52.533 | 20.706 | 337.530 | 30.641 | 52.541 | 20.853 |
| aug-cc-pCVXZ| D-T   |                        | 334.795 | 30.794 | 51.582 | 20.527 | 335.704 | 30.860 | 51.601 | 20.639 |
|            | T-Q    |                        | 336.889 | 30.516 | 51.477 | 20.758 | 338.638 | 30.646 | 51.475 | 20.964 |
|            | Q-5    |                        | 336.617 | 30.549 | 51.538 | 20.744 | 338.111 | 30.656 | 51.537 | 20.922 |
|            | 5-6    |                        | 336.756 | 30.555 | 51.427 | 20.734 | ---     | ---     | ---     | ---     |
| aug-pc-n   | 1-2    |                        | 331.978 | 30.827 | 53.137 | 20.586 | 333.924 | 30.970 | 53.143 | 20.807 |
|            | 2-3    |                        | 337.193 | 30.482 | 51.728 | 20.834 | 338.249 | 30.567 | 51.704 | 20.958 |
|            | 3-4    |                        | 337.615 | 30.586 | 50.488 | 20.732 | 338.457 | 30.649 | 50.484 | 20.833 |
| aug-pcS-n  | 1-2    |                        | 339.247 | 30.834 | 51.181 | 20.610 | 341.122 | 30.968 | 51.188 | 20.832 |
|            | 2-3    |                        | 336.014 | 30.536 | 50.674 | 20.770 | 337.069 | 30.627 | 50.640 | 20.892 |
|            | 3-4    |                        | 337.207 | 30.606 | 50.825 | 20.713 | 338.099 | 30.673 | 50.822 | 20.819 |
| Basis sets     | Experimental Geometry (ExpG) | Optimized Geometry (OptG) |
|---------------|------------------------------|---------------------------|
| Series        | Used cardinal numbers       | Shielding | Anisotropy | Shielding | Anisotropy |
|               |                             | O         | H          | O         | H          |
| cc-pVXZ       | D-T                          | 340.158   | 30.986     | 340.668   | 31.025     | 38.481 | 20.657 |
|               | T-Q                          | 338.911   | 30.582     | 339.113   | 30.603     | 49.275 | 20.724 |
|               | Q-5                          | 336.304   | 30.534     | 335.829   | 30.486     | 51.559 | 20.660 |
|               | S-6                          | 337.286   | 30.601     | 336.743   | 30.557     | 51.418 | 20.606 |
| aug-cc-pVXZ   | D-T                          | 335.568   | 30.853     | 334.535   | 30.766     | 49.890 | 20.386 |
|               | T-Q                          | 338.553   | 30.558     | 338.639   | 30.569     | 49.802 | 20.740 |
|               | Q-5                          | 337.537   | 30.598     | 337.223   | 30.574     | 50.140 | 20.668 |
|               | S-6                          | 338.077   | 30.601     | 337.595   | 30.563     | 49.812 | 20.642 |
| cc-pCVXZ      | D-T                          | 340.802   | 30.934     | 341.775   | 31.009     | 40.535 | 20.714 |
|               | T-Q                          | 337.926   | 30.554     | 338.401   | 30.591     | 48.394 | 20.750 |
|               | Q-5                          | 335.782   | 30.499     | 335.786   | 30.484     | 52.583 | 20.727 |
|               | S-6                          | 337.257   | 30.567     | 337.130   | 30.551     | 51.375 | 20.662 |
| aug-cc-pCVXZ  | D-T                          | 335.929   | 30.806     | 335.393   | 30.757     | 50.260 | 20.446 |
|               | T-Q                          | 337.872   | 30.528     | 338.278   | 30.559     | 50.287 | 20.772 |
|               | Q-5                          | 337.606   | 30.563     | 337.747   | 30.570     | 50.342 | 20.731 |
|               | S-6                          | 337.746   | 30.567     | 337.687   | 30.557     | 50.229 | 20.698 |
| aug-pc-n      | 1-2                          | 332.921   | 30.843     | 333.520   | 30.888     | 51.868 | 20.615 |
|               | 2-3                          | 338.251   | 30.493     | 337.975   | 30.480     | 50.486 | 20.768 |
|               | 3-4                          | 338.567   | 30.597     | 338.091   | 30.563     | 49.275 | 20.646 |
| aug-pcS-n     | 1-2                          | 340.096   | 30.851     | 340.725   | 30.892     | 50.005 | 20.646 |
|               | 2-3                          | 337.019   | 30.549     | 336.734   | 30.540     | 49.438 | 20.702 |
|               | 3-4                          | 338.168   | 30.619     | 337.742   | 30.588     | 49.618 | 20.631 |
Tabel S16: HF: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Used cardinal numbers | | | | | | | | | | | |
|-------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Series      |                        | Zero-Point Vibrational Averaged (ZPVA) | Relative to the Optimized Geometry (ZPVC) | Relative to the Experimental Geometry (ExpC) |
|             |                        | O         | H         | O         | H         | O         | H         | O         | H         | O         | H         |
| cc-pVXZ     | D-T                    | 329.865   | 30.774    | 45.868    | 21.183    | -9.590    | -0.531    | -1.028    | -0.925    | -0.568    | 0.168    | -1.517    | 0.062    |
|             | T-Q                    | 327.097   | 30.569    | 55.831    | 21.023    | -10.445   | -0.514    | -0.896    | -0.928    | -1.354    | 0.125    | -1.583    | 0.065    |
|             | Q-5                    | 324.111   | 30.495    | 58.050    | 21.017    | -10.337   | -0.515    | -0.889    | -0.927    | -1.543    | 0.098    | -1.433    | 0.028    |
|             | 5-6                    | 325.352   | 30.546    | 57.191    | 20.989    | -10.532   | -0.519    | -0.856    | -0.927    | -1.673    | 0.099    | -1.636    | 0.024    |
| aug-cc-pVXZ | D-T                    | 323.681   | 30.663    | 56.714    | 20.909    | -9.980    | -0.530    | -1.106    | -0.911    | -1.560    | 0.100    | -1.556    | -0.024   |
|             | T-Q                    | 327.070   | 30.557    | 55.631    | 21.047    | -10.460   | -0.512    | -0.832    | -0.939    | -1.342    | 0.129    | -1.640    | 0.056    |
|             | Q-5                    | 325.606   | 30.551    | 56.138    | 21.028    | -10.513   | -0.515    | -0.900    | -0.931    | -1.601    | 0.107    | -1.601    | 0.029    |
|             | 5-6                    | 326.163   | 30.545    | 55.828    | 21.018    | -10.396   | -0.517    | -0.912    | -0.930    | -1.600    | 0.102    | -1.595    | 0.024    |
| aug-pc-n    | 1-2                    | 322.048   | 30.710    | 58.313    | 21.100    | -10.422   | -0.524    | -0.710    | -0.945    | -0.354    | 0.187    | -1.452    | 0.106    |
|             | 2-3                    | 326.685   | 30.462    | 56.089    | 21.133    | -10.315   | -0.512    | -1.067    | -0.923    | -1.622    | 0.101    | -1.766    | 0.036    |
|             | 3-4                    | 326.812   | 30.542    | 55.445    | 21.015    | -10.211   | -0.518    | -0.846    | -0.930    | -1.509    | 0.099    | -1.529    | 0.020    |
| aug-pcS-n   | 1-2                    | 330.222   | 30.763    | 55.687    | 21.110    | -10.325   | -0.515    | -0.861    | -0.934    | -0.437    | 0.192    | -1.786    | 0.128    |
|             | 2-3                    | 325.134   | 30.495    | 55.546    | 21.070    | -10.378   | -0.521    | -0.861    | -0.928    | -1.667    | 0.095    | -1.539    | 0.021    |
|             | 3-4                    | 326.250   | 30.567    | 55.706    | 20.991    | -10.383   | -0.517    | -0.898    | -0.928    | -1.594    | 0.103    | -1.580    | 0.023    |
Tabel S17: B3LYP: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Used cardinal numbers | Zero-Point Vibrational Averaged (ZPVA) | Relative to the Optimized Geometry (ZPVC) | Relative to the Experimental Geometry (ExpC) |
|------------|------------------------|----------------------------------------|------------------------------------------|-------------------------------------------|
|            |                        | Σ (Δσ)                                 | σ (Δσ)                                   | σ (Δσ)                                    |
|            |                        | O          | H | O  | H | O       | H      | O       | H  | O       | H  |
| cc-pVXZ   | D-T                    | 319.257    | 30.668 | 37.700 | 18.834 | -12.488 | -0.524 | -2.256 | -1.060 | -12.881 | -0.629 | -2.044 | -1.111 |
|           | T-Q                    | 313.668    | 30.392 | 51.671 | 18.612 | -13.269 | -0.507 | -2.263 | -1.048 | -14.551 | -0.634 | -2.065 | -1.180 |
|           | Q-5                    | 310.024    | 30.230 | 55.677 | 18.645 | -12.806 | -0.506 | -2.221 | -1.032 | -14.552 | -0.678 | -1.964 | -1.206 |
|           | 5-6                    | 310.577    | 30.323 | 55.758 | 18.546 | -12.937 | -0.510 | -2.297 | -1.040 | -14.760 | -0.676 | -2.054 | -1.220 |
| aug-cc-pVXZ | D-T            | 310.405    | 30.451 | 53.439 | 18.548 | -12.641 | -0.521 | -2.380 | -1.036 | -14.544 | -0.711 | -2.130 | -1.216 |
|           | T-Q                    | 312.839    | 30.344 | 53.661 | 18.612 | -13.209 | -0.510 | -2.121 | -1.047 | -14.652 | -0.645 | -1.899 | -1.193 |
|           | Q-5                    | 311.119    | 30.325 | 54.162 | 18.609 | -13.171 | -0.508 | -2.247 | -1.048 | -14.911 | -0.666 | -2.019 | -1.220 |
|           | 5-6                    | 311.555    | 30.325 | 53.703 | 18.588 | -13.237 | -0.511 | -2.338 | -1.049 | -15.010 | -0.672 | -2.118 | -1.226 |
| aug-pc-n  | 1-2                    | 308.782    | 30.489 | 55.927 | 18.633 | -13.044 | -0.517 | -1.947 | -1.055 | -13.941 | -0.626 | -1.655 | -1.138 |
|           | 2-3                    | 312.013    | 30.261 | 53.867 | 18.727 | -13.142 | -0.508 | -2.327 | -1.046 | -14.760 | -0.658 | -2.120 | -1.209 |
|           | 3-4                    | 312.440    | 30.320 | 52.313 | 18.600 | -12.624 | -0.514 | -3.579 | -1.041 | -14.420 | -0.676 | -3.355 | -1.220 |
| aug-pcS-n | 1-2                    | 315.724    | 30.506 | 53.747 | 18.686 | -12.951 | -0.508 | -2.137 | -1.043 | -13.731 | -0.616 | -1.924 | -1.113 |
|           | 2-3                    | 310.560    | 30.289 | 53.393 | 18.648 | -13.185 | -0.514 | -2.180 | -1.048 | -14.964 | -0.672 | -1.968 | -1.228 |
|           | 3-4                    | 311.842    | 30.347 | 53.541 | 18.558 | -13.129 | -0.505 | -2.329 | -1.057 | -14.917 | -0.667 | -2.107 | -1.236 |
Tabel S18: MP2: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Used cardinal numbers | Zero-Point Vibrational Averaged (ZPVA) | Relative to the Optimized Geometry (ZPVC) | Relative to the Experimental Geometry (ExpC) |
|------------|-----------------------|----------------------------------------|------------------------------------------|------------------------------------------|
|            |                       | σ | Δσ | σ | Δσ | σ | Δσ | σ | Δσ |
|            |                       | O | H | O | H | O | H | O | H |
| cc-pVXZ    | D-T                   | 340.111 | 30.268 | 29.864 | 20.125 | -8.670 | -0.524 | -3.040 | -0.964 | -8.247 | -0.482 | -3.284 | -0.928 |
|            | T-Q                   | 338.120 | 29.875 | 41.704 | 20.169 | -9.049 | -0.512 | -2.705 | -0.969 | -8.826 | -0.480 | -2.691 | -0.941 |
|            | Q-5                   | 335.050 | 29.721 | 44.497 | 20.135 | -8.762 | -0.512 | -2.634 | -0.956 | -9.167 | -0.554 | -2.648 | -1.011 |
|            | 5-6                   | 335.653 | 29.790 | 44.608 | 20.079 | -9.001 | -0.515 | -2.624 | -0.952 | -9.486 | -0.557 | -2.656 | -1.017 |
| aug-cc-pVXZ| D-T                   | 333.744 | 30.009 | 42.579 | 19.881 | -8.733 | -0.519 | -2.940 | -0.938 | -9.604 | -0.599 | -3.068 | -1.044 |
|            | T-Q                   | 337.494 | 29.824 | 42.819 | 20.182 | -9.034 | -0.514 | -2.566 | -0.973 | -8.957 | -0.495 | -2.562 | -0.968 |
|            | Q-5                   | 336.326 | 29.811 | 43.059 | 20.138 | -8.978 | -0.513 | -2.680 | -0.968 | -9.237 | -0.532 | -2.706 | -1.003 |
|            | 5-6                   | 336.718 | 29.795 | 42.743 | 20.118 | -8.936 | -0.513 | -2.655 | -0.958 | -9.380 | -0.550 | -2.690 | -1.019 |
| cc-pCVXZ   | D-T                   | 340.947 | 30.257 | 32.321 | 20.188 | -8.905 | -0.523 | -2.904 | -0.963 | -8.018 | -0.437 | -3.005 | -0.862 |
|            | T-Q                   | 337.431 | 29.859 | 40.810 | 20.193 | -8.910 | -0.512 | -2.653 | -0.968 | -8.460 | -0.466 | -2.635 | -0.909 |
|            | Q-5                   | 334.724 | 29.720 | 45.777 | 20.201 | -8.817 | -0.512 | -2.551 | -0.955 | -8.791 | -0.518 | -2.512 | -0.950 |
|            | 5-6                   | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| aug-cc-pCVXZ| D-T                   | 334.357 | 30.001 | 43.239 | 19.942 | -8.924 | -0.521 | -2.769 | -0.940 | -9.321 | -0.558 | -2.805 | -0.982 |
|            | T-Q                   | 337.067 | 29.812 | 43.377 | 20.216 | -8.985 | -0.513 | -2.558 | -0.971 | -8.624 | -0.474 | -2.538 | -0.927 |
|            | Q-5                   | 336.712 | 29.807 | 43.442 | 20.201 | -8.970 | -0.513 | -2.561 | -0.964 | -8.824 | -0.501 | -2.550 | -0.946 |
|            | 5-6                   | 336.672 | 29.789 | 43.295 | 20.170 | -8.956 | -0.515 | -2.583 | -0.963 | -9.015 | -0.521 | -2.584 | -0.971 |
| aug-pc-n   | 1-2                   | 332.304 | 30.127 | 45.239 | 20.089 | -9.036 | -0.520 | -2.454 | -0.969 | -8.385 | -0.459 | -2.418 | -0.887 |
|            | 2-3                   | 336.849 | 29.754 | 43.233 | 20.221 | -9.032 | -0.510 | -2.881 | -0.964 | -9.207 | -0.510 | -2.946 | -0.993 |
|            | 3-4                   | 337.198 | 29.804 | 42.262 | 20.113 | -8.923 | -0.514 | -2.595 | -0.967 | -9.317 | -0.542 | -2.646 | -1.023 |
| aug-pcS-n  | 1-2                   | 339.495 | 30.144 | 43.176 | 20.126 | -8.915 | -0.508 | -2.601 | -0.958 | -8.265 | -0.452 | -2.553 | -0.872 |
|            | 2-3                   | 335.618 | 29.796 | 42.288 | 20.150 | -9.058 | -0.520 | -2.720 | -0.969 | -9.265 | -0.516 | -2.802 | -1.003 |
|            | 3-4                   | 336.836 | 29.828 | 42.581 | 20.100 | -8.949 | -0.515 | -2.618 | -0.965 | -9.298 | -0.542 | -2.663 | -1.014 |
Tabel S19: CCSD: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

| Basis sets | Series | Zero-Point Vibrational Averaged (ZPVA) | Relative to the Optimized Geometry (ZPVC) | Relative to the Experimental Geometry (ExpC) |
|------------|--------|----------------------------------------|------------------------------------------|------------------------------------------|
|            |        | σ | Δσ | σ | O | H | O | H | σ | O | H | O | H | O | H | O | H | σ | O | H | O | H |
| cc-pVXZ    | D-T    | 330.458 | 30.563 | 37.929 | 19.832 | -10.241 | -0.522 | -2.190 | -1.004 | -8.552 | -0.394 | -2.324 | -0.820 |
|            | T-Q    | 328.519 | 30.175 | 48.825 | 19.895 | -10.779 | -0.507 | -1.864 | -1.012 | -9.284 | -0.392 | -1.833 | -0.834 |
|            | Q-5    | 325.554 | 30.073 | 50.990 | 19.846 | -10.603 | -0.505 | -1.839 | -1.001 | -9.744 | -0.452 | -1.782 | -0.897 |
|            | 5-6    | 326.360 | 30.136 | 50.690 | 19.792 | -10.793 | -0.508 | -1.858 | -1.002 | -9.992 | -0.455 | -1.857 | -0.909 |
| aug-cc-pVXZ| D-T    | 324.354 | 30.349 | 49.052 | 19.587 | -10.467 | -0.514 | -2.172 | -0.984 | -10.137 | -0.492 | -2.179 | -0.940 |
|            | T-Q    | 328.207 | 30.145 | 49.194 | 19.910 | -10.774 | -0.509 | -1.779 | -1.015 | -9.386 | -0.401 | -1.779 | -0.852 |
|            | Q-5    | 326.825 | 30.152 | 49.439 | 19.845 | -10.763 | -0.506 | -1.900 | -1.012 | -9.752 | -0.434 | -1.899 | -0.892 |
|            | 5-6    | 327.330 | 30.149 | 49.138 | 19.835 | -10.620 | -0.500 | -1.873 | -0.995 | -9.783 | -0.438 | -1.866 | -0.894 |
| cc-pCVXZ   | D-T    | 331.345 | 30.556 | 40.097 | 19.899 | -10.473 | -0.520 | -2.062 | -1.005 | -8.234 | -0.351 | -2.120 | -0.753 |
|            | T-Q    | 327.999 | 30.165 | 48.034 | 19.929 | -10.611 | -0.506 | -1.814 | -1.008 | -8.808 | -0.371 | -1.791 | -0.795 |
|            | Q-5    | 325.529 | 30.073 | 52.041 | 19.917 | -10.614 | -0.506 | -1.768 | -1.001 | -9.235 | -0.417 | -1.721 | -0.834 |
|            | 5-6    | ---    | ---   | 50.749 | 19.555 | ---    | ---   | -1.792 | -1.298 | ---    | ---   | -1.784 | -1.150 |
| aug-cc-pCVXZ| D-T    | 325.062 | 30.345 | 49.591 | 19.655 | -10.642 | -0.515 | -2.009 | -0.984 | -9.734 | -0.449 | -1.991 | -0.872 |
|            | T-Q    | 327.939 | 30.138 | 49.700 | 19.951 | -10.699 | -0.508 | -1.774 | -1.013 | -8.950 | -0.378 | -1.776 | -0.808 |
|            | Q-5    | 327.388 | 30.150 | 49.743 | 19.913 | -10.723 | -0.506 | -1.794 | -1.009 | -9.229 | -0.399 | -1.794 | -0.832 |
|            | 5-6    | ---    | ---   | ---    | ---   | ---    | ---   | ---    | ---   | ---    | ---   | ---    | ---   |
| aug-pc-n   | 1-2    | 323.119 | 30.453 | 51.403 | 19.787 | -10.805 | -0.517 | -1.741 | -1.020 | -8.859 | -0.374 | -1.735 | -0.799 |
|            | 2-3    | 327.452 | 30.065 | 49.644 | 19.946 | -10.797 | -0.502 | -2.059 | -1.012 | -9.742 | -0.417 | -2.084 | -0.888 |
|            | 3-4    | 327.778 | 30.148 | 48.594 | 19.824 | -10.680 | -0.502 | -1.891 | -1.009 | -9.838 | -0.439 | -1.894 | -0.908 |
| aug-pcS-n  | 1-2    | 330.470 | 30.465 | 49.308 | 19.825 | -10.652 | -0.504 | -1.880 | -1.007 | -8.776 | -0.369 | -1.872 | -0.785 |
|            | 2-3    | 326.248 | 30.116 | 48.782 | 19.877 | -10.821 | -0.510 | -1.857 | -1.016 | -9.767 | -0.420 | -1.892 | -0.893 |
|            | 3-4    | 327.285 | 30.161 | 48.815 | 19.979 | -10.814 | -0.512 | -2.008 | -1.022 | -9.922 | -0.446 | -2.010 | -0.916 |
## Tabel S20: CCSD(T): extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

| Basis sets     |  |  |  | Zero-Point Vibrational |  |  |  | Relative to the Optimized Geometry |  |  |  | Relative to the Experimental Geometry |  |
|----------------|---|---|---|--------------------------|---|---|---|------------------------------------|---|---|---|--------------------------------------|---|
|                | Series |  Δσ | σ | O | H | O | H | Δσ | σ | O | H | Δσ | σ | O | H | Δσ | σ | O | H | Δσ | σ | O | H |
|                | cc-pVXZ | D-T | 330.172 | 30.503 | 35.978 | 19.627 | -10.496 | -0.522 | -2.503 | -1.029 | -9.986 | -0.483 | -2.720 | -0.986 | |
|                |        | T-Q | 328.116 | 30.096 | 47.122 | 19.690 | -10.997 | -0.507 | -2.154 | -1.034 | -10.795 | -0.486 | -2.123 | -1.011 | |
|                |        | Q-5 | 325.024 | 29.979 | 49.444 | 19.640 | -10.805 | -0.507 | -2.115 | -1.021 | -11.280 | -0.555 | -2.088 | -1.078 | |
|                |        | 5-6 | 325.730 | 30.045 | 49.279 | 19.582 | -11.014 | -0.511 | -2.139 | -1.024 | -11.557 | -0.556 | -2.128 | -1.086 | |
|                | aug-cc-pVXZ | D-T | 323.875 | 30.252 | 47.424 | 19.381 | -10.661 | -0.514 | -2.466 | -1.005 | -11.693 | -0.601 | -2.534 | -1.118 | |
|                |        | T-Q | 327.643 | 30.059 | 47.746 | 19.702 | -10.995 | -0.510 | -2.056 | -1.038 | -10.910 | -0.498 | -2.035 | -1.032 | |
|                |        | Q-5 | 326.232 | 30.065 | 47.959 | 19.636 | -10.991 | -0.509 | -2.181 | -1.032 | -11.305 | -0.533 | -2.180 | -1.070 | |
|                |        | 5-6 | 326.617 | 30.057 | 47.675 | 19.611 | -10.978 | -0.506 | -2.137 | -1.030 | -11.460 | -0.544 | -2.136 | -1.089 | |
|                | cc-pCVXZ | D-T | 331.037 | 30.489 | 48.145 | 19.684 | -10.738 | -0.520 | -2.389 | -1.030 | -9.765 | -0.445 | -2.498 | -0.926 | |
|                |        | T-Q | 327.569 | 30.083 | 46.289 | 19.719 | -10.832 | -0.507 | -2.105 | -1.031 | -10.357 | -0.471 | -2.080 | -0.976 | |
|                |        | Q-5 | 324.974 | 29.977 | 50.533 | 19.707 | -10.812 | -0.507 | -2.050 | -1.021 | -10.808 | -0.522 | -1.994 | -1.019 | |
|                |        | 5-6 |       |       |       |       |       |       |       |       |       |       |       |       | |
|                | aug-cc-pCVXZ | D-T | 324.550 | 30.242 | 47.945 | 19.439 | -10.843 | -0.514 | -2.315 | -1.007 | -11.379 | -0.564 | -2.321 | -1.059 | |
|                |        | T-Q | 327.355 | 30.050 | 48.233 | 19.737 | -10.923 | -0.508 | -2.054 | -1.035 | -10.517 | -0.477 | -2.032 | -0.991 | |
|                |        | Q-5 | 326.794 | 30.060 | 48.265 | 19.698 | -10.953 | -0.510 | -2.077 | -1.033 | -10.812 | -0.503 | -2.060 | -1.015 | |
|                |        | 5-6 | 326.668 | 30.039 | 48.171 | 19.661 | -11.019 | -0.518 | -2.057 | -1.037 | -11.078 | -0.527 | -2.044 | -1.044 | |
|                | aug-pc-n | 1-2 | 322.506 | 30.370 | 49.824 | 19.575 | -11.015 | -0.518 | -2.044 | -1.040 | -10.416 | -0.473 | -2.039 | -0.975 | |
|                |        | 2-3 | 326.979 | 29.979 | 48.080 | 19.735 | -10.996 | -0.501 | -2.406 | -1.033 | -11.271 | -0.514 | -2.441 | -1.070 | |
|                |        | 3-4 | 327.331 | 30.070 | 47.306 | 19.626 | -10.760 | -0.494 | -1.969 | -1.020 | -11.236 | -0.528 | -1.979 | -1.078 | |
|                | aug-pc5-n | 1-2 | 327.858 | 30.388 | 47.845 | 19.620 | -10.867 | -0.505 | -2.160 | -1.026 | -10.238 | -0.463 | -2.130 | -0.951 | |
|                |        | 2-3 | 325.656 | 30.028 | 47.251 | 19.661 | -11.078 | -0.511 | -2.187 | -1.041 | -11.363 | -0.520 | -2.239 | -1.079 | |
|                |        | 3-4 | 326.883 | 30.081 | 47.472 | 19.604 | -10.859 | -0.507 | -2.146 | -1.027 | -11.285 | -0.539 | -2.150 | -1.078 | |
### Tabel S21: HF: extrapolated shieldings using the exponential function and specified basis sets

| Basis sets | Optimized Geometry (OptG) | Zero-Point Vibrational Averaged (ZPVA) |
|------------|---------------------------|----------------------------------------|
| Series     | Used cardinal numbers     | Shielding                              | Shielding                              |
|            |                           | O H                                    | O H                                    |
| aug-cc-pVXZ| D-Q                       | 337.150 31.052                         | 326.848 30.556                         |
|            | T-5                       | 336.931 31.093                         | 326.664 30.575                         |
|            | Q-6                       | 336.615 31.075                         | 326.210 30.557                         |
| aug-pcS-n  | 2-4                       | 336.932 31.110                         | 326.533 30.597                         |
|            | 3-5                       | 336.625 31.084                         | 326.239 30.567                         |

### Tabel S22: CCSD(T): extrapolated shieldings using the exponential function and specified basis sets

| Basis sets | Optimized Geometry (OptG) | Zero-Point Vibrational Averaged (ZPVA) |
|------------|---------------------------|----------------------------------------|
| Series     | Used cardinal numbers     | Shielding                              | Shielding                              |
|            |                           | O H                                    | O H                                    |
| aug-cc-pCVXZ| D-Q                       | 337.622 30.433                         | 326.646 29.932                         |
|            | T-5                       | 337.744 30.606                         | 326.791 30.095                         |
|            | Q-6                       | 337.741 30.567                         | 326.788 30.039                         |
| aug-pcS-n  | 2-4                       | 337.484 30.709                         | 326.412 30.208                         |
|            | 3-5                       | 337.521 30.612                         | 326.518 30.105                         |