

Supplementary Material

Accurate Born-Oppenheimer potentials for excited Σ^+ states of the hydrogen molecule

Michał Silkowski, Magdalena Zientkiewicz, Krzysztof Pachucki
Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland
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For additional quantities and operators, such as dE/dR , $-\langle\nabla_1^2\rangle/2$ and $-\langle\nabla_1 \cdot \nabla_2\rangle/2$ along with E itself, we refer to the plain text format of the Supplementary Material.

Table S1: Calculated BO energies of the $2^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$2^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.316 515 768 616 4(4)	4.3	-0.714 395 560 089 51(2)
0.8	-0.436 425 593 131 4(2)	4.4	-0.714 520 556 251 95(7)
0.9	-0.520 350 468 544 3(2)	4.5	-0.714 350 459 119 94(9)
1.0	-0.580 085 582 389 8(2)	4.6	-0.713 919 923 180 97(7)
1.1	-0.623 016 874 818 74(8)	4.7	-0.713 261 360 033 09(7)
1.2	-0.653 971 526 522 602(3)	4.8	-0.712 404 663 601 50(9)
1.3	-0.676 214 704 985 28(3)	4.9	-0.711 377 111 823 75(9)
1.4	-0.692 018 180 995 9(5)	5.0	-0.710 203 383 787 87(9)
1.5	-0.703 000 247 099 5(10)	5.1	-0.708 905 651 343 38(9)
1.6	-0.710 336 982 657 7(2)	5.2	-0.707 503 716 943 88(9)
1.7	-0.714 897 955 305 9(3)	5.3	-0.706 015 177 995 18(9)
1.8	-0.717 335 894 340 5(7)	5.4	-0.704 455 603 904 74(9)
1.9	-0.718 147 445 823 35(6)	5.5	-0.702 838 716 262 41(9)
2.0	-0.717 715 279 148 71(3)	5.6	-0.701 176 565 656 23(9)
2.1	-0.716 337 913 674 15(3)	5.7	-0.699 479 700 871 81(9)
2.2	-0.714 251 348 494 99(6)	5.8	-0.697 757 327 857 6(2)
2.3	-0.711 645 225 229 490(8)	5.9	-0.696 017 457 017 1(2)
2.4	-0.708 675 480 663 436(5)	6.0	-0.694 267 038 224 6(6)
2.5	-0.705 475 096 655 70(2)	6.5	-0.685 540 216 160 06(8)
2.6	-0.702 164 628 697 69(2)	7.0	-0.677 165 653 649 0(2)
2.7	-0.698 864 888 169 62(7)	7.5	-0.669 365 631 391 96(8)
2.8	-0.695 715 952 317 034(8)	8.0	-0.662 221 029 584(2)
2.9	-0.692 910 056 096 402(4)	8.5	-0.655 747 598 735(2)
3.0	-0.690 747 056 393 04(3)	9.0	-0.649 936 081 568(2)
3.1	-0.689 687 377 420 23(5)	9.5	-0.644 773 573 844(2)
3.2	-0.690 223 260 674 9(2)	10.0	-0.640 254 776 824(2)
3.3	-0.692 387 458 811 5(2)	11.0	-0.633 180 755 609 1(10)
3.4	-0.695 573 423 188 2(2)	12.0	-0.628 742 126 229 3(5)
3.5	-0.699 079 703 707 33(9)	13.0	-0.626 498 816 980 3(4)
3.6	-0.702 460 667 995 92(7)	14.0	-0.625 556 093 240 1(2)
3.7	-0.705 495 303 750 75(5)	15.0	-0.625 203 014 128 99(9)
3.8	-0.708 090 170 985 61(3)	16.0	-0.625 079 154 799 58(5)
3.9	-0.710 217 777 471 76(2)	17.0	-0.625 034 674 818 94(3)
4.0	-0.711 884 509 253 60(2)	18.0	-0.625 017 096 934 63(2)
4.1	-0.713 114 152 789 37(2)	19.0	-0.625 009 376 716 31(2)
4.2	-0.713 939 118 843 68(2)	20.0	-0.625 005 640 453 183(4)

Table S2: Calculated BO energies of the $3^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$3^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.240 521 729 67(3)	4.3	-0.641 845 665 471 78(9)
0.8	-0.361 818 601 10(6)	4.4	-0.639 999 584 864 7(1)
0.9	-0.447 069 355 88(2)	4.5	-0.638 295 632 428 1(6)
1.0	-0.508 066 130 356(8)	4.6	-0.636 732 643 288 28(8)
1.1	-0.552 582 069 001(2)	4.7	-0.635 307 374 134 00(7)
1.2	-0.585 253 000 503 92(8)	4.8	-0.634 014 937 713 46(9)
1.3	-0.609 140 059 040 39(7)	4.9	-0.632 849 164 400 33(8)
1.4	-0.626 518 022 757 26(4)	5.0	-0.631 802 920 887 66(7)
1.5	-0.639 008 659 587 76(5)	5.1	-0.630 868 399 028 46(7)
1.6	-0.647 791 886 695 31(2)	5.2	-0.630 037 378 141 54(6)
1.7	-0.653 741 492 555 054(2)	5.3	-0.629 301 459 242 97(5)
1.8	-0.657 514 963 179 179(4)	5.4	-0.628 652 268 058 24(6)
1.9	-0.659 614 566 278 383(5)	5.5	-0.628 081 624 122 65(5)
2.0	-0.660 430 067 353 057(7)	5.6	-0.627 581 674 824 80(5)
2.1	-0.660 269 664 591 789(7)	5.7	-0.627 144 995 145 93(4)
2.2	-0.659 383 681 634 108(8)	5.8	-0.626 764 655 583 50(6)
2.3	-0.657 984 730 816 22(2)	5.9	-0.626 434 262 034 26(6)
2.4	-0.656 268 502 287 25(2)	6.0	-0.626 147 972 151 88(5)
2.5	-0.654 441 798 941 61(2)	6.5	-0.625 210 860 843 65(4)
2.6	-0.652 770 242 259 41(4)	7.0	-0.624 784 653 394 07(3)
2.7	-0.651 662 396 869 6(2)	7.5	-0.624 609 143 198 78(3)
2.8	-0.651 749 600 058 2(5)	8.0	-0.624 553 270 901 82(2)
2.9	-0.653 626 409 721 4(4)	8.5	-0.624 552 621 321 99(2)
3.0	-0.656 985 952 465(4)	9.0	-0.624 575 830 346 187(9)
3.1	-0.660 470 206 304(4)	9.5	-0.624 607 741 026 967(9)
3.2	-0.662 692 422 119 4(9)	10.0	-0.624 641 136 009 254(9)
3.3	-0.663 103 508 233 3(10)	11.0	-0.624 700 931 500 543(7)
3.4	-0.662 070 328 565 9(2)	12.0	-0.624 745 654 032 564(8)
3.5	-0.660 201 941 028 55(6)	13.0	-0.624 774 071 241 936(8)
3.6	-0.657 925 762 916 8(4)	14.0	-0.624 786 718 142 81(2)
3.7	-0.655 482 082 108 2(5)	15.0	-0.624 788 947 082 67(2)
3.8	-0.653 002 475 032(1)	16.0	-0.624 793 681 978 11(2)
3.9	-0.650 561 527 216 2(2)	17.0	-0.624 807 739 272 856(1)
4.0	-0.648 203 357 002 5(5)	18.0	-0.624 827 450 746 38(2)
4.1	-0.645 954 837 686 47(10)	19.0	-0.624 848 071 538 2(9)
4.2	-0.643 832 394 170 64(9)	20.0	-0.624 867 158 264 172(3)

Table S3: Calculated BO energies of the $4^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$4^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.238 469 687 512 3(7)	4.3	-0.599 537 485 842 4(4)
0.8	-0.360 391 556 326 5(2)	4.4	-0.597 731 052 126 3(3)
0.9	-0.446 257 979 308 4(3)	4.5	-0.596 041 711 437 1(3)
1.0	-0.507 859 815 261 01(7)	4.6	-0.594 468 203 035 1(4)
1.1	-0.552 194 141 040 3(6)	4.7	-0.593 008 641 414 4(4)
1.2	-0.584 281 145 968 8(9)	4.8	-0.591 660 754 131 4(3)
1.3	-0.607 593 563 246 9(4)	4.9	-0.590 422 095 837 9(3)
1.4	-0.624 404 699 845 8(3)	5.0	-0.589 290 231 443 9(6)
1.5	-0.636 334 418 752 0(2)	5.1	-0.588 262 880 193 1(3)
1.6	-0.644 560 234 044 5(2)	5.2	-0.587 338 013 713 3(3)
1.7	-0.649 952 886 803 4(2)	5.3	-0.586 513 903 938 7(4)
1.8	-0.653 165 913 043 9(5)	5.4	-0.585 789 120 428 3(3)
1.9	-0.654 696 295 339 2(2)	5.5	-0.585 162 480 220 7(3)
2.0	-0.654 926 452 522 1(2)	5.6	-0.584 632 956 657 9(4)
2.1	-0.654 153 921 660 3(3)	5.7	-0.584 199 556 399 0(4)
2.2	-0.652 612 802 430 7(2)	5.8	-0.583 861 176 146 2(3)
2.3	-0.650 489 688 913 73(9)	5.9	-0.583 616 452 359 0(3)
2.4	-0.647 936 073 910 20(9)	6.0	-0.583 463 618 207 5(3)
2.5	-0.645 078 974 518 13(8)	6.5	-0.583 975 483 001 2(5)
2.6	-0.642 031 942 126 9(2)	7.0	-0.586 185 060 781(3)
2.7	-0.638 910 077 808 2(4)	7.5	-0.589 360 449 965(2)
2.8	-0.635 853 597 599 2(1)	8.0	-0.592 843 558 852 3(3)
2.9	-0.633 040 236 390 5(2)	8.5	-0.596 188 935 044 4(3)
3.0	-0.630 554 138 785 5(2)	9.0	-0.599 141 965 037 3(5)
3.1	-0.628 188 893 749 9(9)	9.5	-0.601 572 505 312 6(2)
3.2	-0.625 732 220 558 4(3)	10.0	-0.603 417 899 168 2(8)
3.3	-0.623 163 584 624 9(3)	11.0	-0.605 241 805 347 7(9)
3.4	-0.620 535 305 447 0(2)	12.0	-0.604 584 452 519(2)
3.5	-0.617 899 875 102 8(3)	13.0	-0.601 971 058 000(2)
3.6	-0.615 296 728 245 1(3)	14.0	-0.598 366 964 57(2)
3.7	-0.612 753 869 356 7(2)	15.0	-0.594 515 996 73(2)
3.8	-0.610 291 046 089 6(6)	16.0	-0.590 775 653 672(7)
3.9	-0.607 922 173 312 5(6)	17.0	-0.587 279 963 997 3(3)
4.0	-0.605 656 958 283 3(3)	18.0	-0.584 065 109 045(5)
4.1	-0.603 501 974 500 1(3)	19.0	-0.581 127 641 784(7)
4.2	-0.601 461 389 922 5(3)	20.0	-0.578 449 007 347(9)

Table S4: Calculated BO energies of the $5^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$5^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.214 825 011 937(5)	4.3	-0.587 453 175 649 1(2)
0.8	-0.336 447 866 470(5)	4.4	-0.585 261 684 172 0(2)
0.9	-0.422 012 812 363(5)	4.5	-0.583 192 634 594 0(2)
1.0	-0.483 310 990 124(4)	4.6	-0.581 243 982 248 0(2)
1.1	-0.527 931 910 869 4(7)	4.7	-0.579 413 005 133 2(2)
1.2	-0.560 542 400 786 1(5)	4.8	-0.577 696 421 046 3(2)
1.3	-0.584 362 217 874 7(5)	4.9	-0.576 090 491 514 0(2)
1.4	-0.601 665 497 322 7(4)	5.0	-0.574 591 113 727 5(2)
1.5	-0.614 073 206 566 5(3)	5.1	-0.573 193 900 685 9(2)
1.6	-0.622 764 258 272 5(3)	5.2	-0.571 894 249 709 6(2)
1.7	-0.628 611 169 116 9(2)	5.3	-0.570 687 400 032 9(2)
1.8	-0.632 269 800 199 0(2)	5.4	-0.569 568 480 982 6(3)
1.9	-0.634 240 327 287 6(2)	5.5	-0.568 532 552 970 6(2)
2.0	-0.634 909 814 936 9(2)	5.6	-0.567 574 643 953 8(2)
2.1	-0.634 583 006 839 7(3)	5.7	-0.566 689 784 012 2(2)
2.2	-0.633 505 990 241 4(2)	5.8	-0.565 873 040 247 1(6)
2.3	-0.631 886 891 869 2(2)	5.9	-0.565 119 553 391 2(5)
2.4	-0.629 919 339 992 7(3)	6.0	-0.564 424 576 465 0(5)
2.5	-0.627 820 691 240 6(6)	6.5	-0.561 673 973 796 7(2)
2.6	-0.625 911 872 660(2)	7.0	-0.559 799 903 937 23(7)
2.7	-0.624 738 854 739(2)	7.5	-0.558 491 460 092 84(9)
2.8	-0.624 751 807 635(2)	8.0	-0.557 571 402 514 3(2)
2.9	-0.624 975 673 540(2)	8.5	-0.556 931 100 601 9(3)
3.0	-0.623 922 761 636 2(10)	9.0	-0.556 492 993 256 3(3)
3.1	-0.621 624 545 371 6(5)	9.5	-0.556 197 803 667 92(2)
3.2	-0.618 723 067 237 5(3)	10.0	-0.556 000 846 895 6(2)
3.3	-0.615 600 289 196 4(3)	11.0	-0.555 782 206 035 42(10)
3.4	-0.612 422 395 299(2)	12.0	-0.555 682 256 514 32(3)
3.5	-0.609 265 909 824 9(3)	13.0	-0.555 632 969 518 38(3)
3.6	-0.606 171 018 911 9(3)	14.0	-0.555 606 161 677 62(5)
3.7	-0.603 161 346 099 1(2)	15.0	-0.555 590 181 110 912(3)
3.8	-0.600 251 866 052 9(2)	16.0	-0.555 579 970 036 133(2)
3.9	-0.597 452 442 986 2(7)	17.0	-0.555 573 133 690 222(5)
4.0	-0.594 769 592 624 1(3)	18.0	-0.555 568 415 321 604(4)
4.1	-0.592 207 448 917 2(3)	19.0	-0.555 565 090 350 473(2)
4.2	-0.589 768 342 517 8(2)	20.0	-0.555 562 710 376 694(2)

Table S5: Calculated BO energies of the $6^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$6^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.214 002 325 509 2(9)	4.3	-0.571 819 715 484(2)
0.8	-0.335 886 648 909(3)	4.4	-0.569 694 733 503 0(10)
0.9	-0.421 710 285 628(2)	4.5	-0.567 684 437 16(3)
1.0	-0.483 263 818 706 8(6)	4.6	-0.565 789 362 518(2)
1.1	-0.527 727 162 319(2)	4.7	-0.564 010 361 903(2)
1.2	-0.560 088 946 762(5)	4.8	-0.562 349 067 676(2)
1.3	-0.583 662 794 181 5(5)	4.9	-0.560 808 486 465(2)
1.4	-0.600 722 125 239 1(4)	5.0	-0.559 393 752 871(2)
1.5	-0.612 886 936 100 8(3)	5.1	-0.558 113 008 001(2)
1.6	-0.621 334 847 930 2(8)	5.2	-0.556 978 160 367(2)
1.7	-0.626 936 644 592 3(4)	5.3	-0.556 004 801 071(2)
1.8	-0.630 345 802 683 5(3)	5.4	-0.555 209 840 020(2)
1.9	-0.632 059 098 539 7(4)	5.5	-0.554 605 475 403(2)
2.0	-0.632 458 537 824 1(5)	5.6	-0.554 190 874 544(2)
2.1	-0.631 840 948 806 5(8)	5.7	-0.553 947 456 853(2)
2.2	-0.630 439 288 017 1(3)	5.8	-0.553 842 750 631(2)
2.3	-0.628 438 346 665 3(3)	5.9	-0.553 839 824 993(8)
2.4	-0.625 986 780 886 8(3)	6.0	-0.553 905 281 146(7)
2.5	-0.623 207 119 465 2(3)	6.5	-0.554 556 616 403(3)
2.6	-0.620 205 806 027 0(2)	7.0	-0.555 073 152 157(2)
2.7	-0.617 086 705 196 3(1)	7.5	-0.555 341 486 986 9(7)
2.8	-0.613 968 242 489 5(8)	8.0	-0.555 463 000 743 28(5)
2.9	-0.610 951 300 507 9(9)	8.5	-0.555 513 990 172 77(2)
3.0	-0.607 984 520 050(2)	9.0	-0.555 533 302 981 43(2)
3.1	-0.604 965 579 196(2)	9.5	-0.555 538 968 714 818(9)
3.2	-0.601 893 387 552(2)	10.0	-0.555 539 184 914 083(7)
3.3	-0.598 806 494 758(2)	11.0	-0.555 535 862 495 673(6)
3.4	-0.595 740 596 378(2)	12.0	-0.555 533 720 966 736(5)
3.5	-0.592 722 480 238(2)	13.0	-0.555 533 653 499 766(3)
3.6	-0.589 771 654 135 5(10)	14.0	-0.555 534 879 773 837(3)
3.7	-0.586 902 363 060 0(7)	15.0	-0.555 536 678 642 624(2)
3.8	-0.584 125 047 623 0(10)	16.0	-0.555 538 626 624 646(5)
3.9	-0.581 447 330 977(2)	17.0	-0.555 540 514 441 146(4)
4.0	-0.578 874 699 33(7)	18.0	-0.555 542 251 438 849(2)
4.1	-0.576 410 993 974 2(10)	19.0	-0.555 543 806 971 529(2)
4.2	-0.574 058 790 625(2)	20.0	-0.555 545 179 435 428(4)

Table S6: Calculated BO energies of the $7^1\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$7^1\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.203 102 622 6(5)	4.3	-0.567 038 119 622 9(6)
0.8	-0.324 839 806 2(2)	4.4	-0.564 803 850 249 7(5)
0.9	-0.410 515 404 90(9)	4.5	-0.562 691 885 771 8(5)
1.0	-0.471 920 166 180(3)	4.6	-0.560 702 734 472 9(4)
1.1	-0.516 552 689 791(8)	4.7	-0.558 837 170 226 8(3)
1.2	-0.549 140 355 703(4)	4.8	-0.557 096 631 169 3(4)
1.3	-0.572 934 607 636(3)	4.9	-0.555 483 706 328 3(3)
1.4	-0.590 209 251 251(3)	5.0	-0.554 002 643 920 4(2)
1.5	-0.602 584 827 761(3)	5.1	-0.552 659 574 586 51(5)
1.6	-0.611 239 689 956(2)	5.2	-0.551 461 557 353 37(5)
1.7	-0.617 045 605 402(2)	5.3	-0.550 412 708 706 57(7)
1.8	-0.620 657 411 113(2)	5.4	-0.549 506 262 085 4(2)
1.9	-0.622 573 847 780(7)	5.5	-0.548 717 036 630 6(5)
2.0	-0.623 179 911 691 0(7)	5.6	-0.548 005 389 356 5(9)
2.1	-0.622 777 271 635 1(8)	5.7	-0.547 334 145 102(2)
2.2	-0.621 607 292 156(4)	5.8	-0.546 682 226 458(9)
2.3	-0.619 870 632 378(2)	5.9	-0.546 044 643 95(2)
2.4	-0.617 748 981 607(3)	6.0	-0.545 425 285 37(2)
2.5	-0.615 441 450 167(6)	6.5	-0.542 800 702 69(7)
2.6	-0.613 242 851 054(4)	7.0	-0.541 166 772 92(5)
2.7	-0.611 586 970 844(8)	7.5	-0.540 389 045 22(5)
2.8	-0.610 297 993 373(6)	8.0	-0.540 117 868 73(5)
2.9	-0.608 278 117 747(2)	8.5	-0.540 057 633 77(4)
3.0	-0.605 439 878 414(2)	9.0	-0.540 063 429 78(5)
3.1	-0.602 241 084 513(2)	9.5	-0.540 095 735 05(3)
3.2	-0.598 932 119 302 7(6)	10.0	-0.540 163 206 44(3)
3.3	-0.595 613 919 087(2)	11.0	-0.540 506 829 23(2)
3.4	-0.592 333 621 394 3(8)	12.0	-0.541 285 873 90(6)
3.5	-0.589 117 978 588 1(8)	13.0	-0.542 568 372 60(7)
3.6	-0.585 984 337 277 6(8)	14.0	-0.544 242 341 19(6)
3.7	-0.582 944 810 275 1(8)	15.0	-0.546 082 002 38(5)
3.8	-0.580 008 156 559 2(7)	16.0	-0.547 871 974 10(10)
3.9	-0.577 180 773 207(2)	17.0	-0.549 476 125 466(10)
4.0	-0.574 467 295 342(4)	18.0	-0.550 836 884 54(2)
4.1	-0.571 871 003 717 3(2)	19.0	-0.551 948 554 63(3)
4.2	-0.569 394 131 578 1(8)	20.0	-0.552 832 564 915(10)

Table S7: Calculated BO energies of the $1^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$1^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.342130928988667(6)	4.3	-0.653195827155049(8)
0.8	-0.46143498347982(4)	4.4	-0.65073706182336(2)
0.9	-0.544767040091894(3)	4.5	-0.6484429623517(4)
1.0	-0.60392224803181505(4)	4.6	-0.6463109963342(4)
1.1	-0.6462856755609065(2)	4.7	-0.644337697996883(3)
1.2	-0.67668314180341571(6)	4.8	-0.6425186973868(9)
1.3	-0.69837814548896884(3)	4.9	-0.64084876299434(10)
1.4	-0.7136405684873686(3)	5.0	-0.639321863500910(9)
1.5	-0.7240866205382896(3)	5.1	-0.637931252052529(10)
1.6	-0.730890086928356(5)	5.2	-0.636669573606577(10)
1.7	-0.734917974883440(1)	5.3	-0.6355289928497(10)
1.8	-0.736820091741595(7)	5.4	-0.634501337399442(10)
1.9	-0.7370896537668271(1)	5.5	-0.63357824894624(3)
2.0	-0.7361051733454439(3)	5.6	-0.6327513339942(6)
2.1	-0.7341599538590402(5)	5.7	-0.6320123060258(5)
2.2	-0.7314832061423001(5)	5.8	-0.63135311211810(10)
2.3	-0.7282553924169136(7)	5.9	-0.63076603896819(2)
2.4	-0.724619525233251(2)	6.0	-0.63024379552804(2)
2.5	-0.720689588359196(4)	6.5	-0.6283849655891246(9)
2.6	-0.716556881346118(10)	7.0	-0.627343969517241(3)
2.7	-0.712294847112937(1)	7.5	-0.6267388331983872(5)
2.8	-0.707962778269134(4)	8.0	-0.6263678024076574(9)
2.9	-0.703608685724174(4)	8.5	-0.626127410224462(2)
3.0	-0.699271535123230(2)	9.0	-0.6259640651384734(9)
3.1	-0.694983001681094(6)	9.5	-0.625848897568859(2)
3.2	-0.6907688547753517(8)	10.0	-0.625765155314512(2)
3.3	-0.6866500553689703(6)	11.0	-0.625651263865481(1)
3.4	-0.6826436287043045(9)	12.0	-0.625565960913511(5)
3.5	-0.6787633595262160(5)	13.0	-0.625485558864006(2)
3.6	-0.675020345825230(2)	14.0	-0.6254088253710753(7)
3.7	-0.6714234386847724(8)	15.0	-0.6253403831152288(4)
3.8	-0.6679795895349028(9)	16.0	-0.6252826990251769(5)
3.9	-0.66469412144608(2)	17.0	-0.62523562891080(2)
4.0	-0.661570937686215(2)	18.0	-0.6251977430164360(2)
4.1	-0.658612678362044(2)	19.0	-0.6251673111090794(2)
4.2	-0.655820834391176(3)	20.0	-0.6251427558519418(1)

Table S8: Calculated BO energies of the $2^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$2^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.247 264 442 604 2(4)	4.3	-0.614 697 062 021 16(2)
0.8	-0.368 441 813 489 63(8)	4.4	-0.613 958 695 445 20(2)
0.9	-0.453 573 150 521 41(2)	4.5	-0.613 364 273 414 49(2)
1.0	-0.514 450 615 877 05(2)	4.6	-0.612 901 703 757 55(2)
1.1	-0.558 459 323 262 524(3)	4.7	-0.612 558 617 305 02(2)
1.2	-0.590 426 867 896 656(9)	4.8	-0.612 322 805 243 64(3)
1.3	-0.613 619 506 234 056(4)	4.9	-0.612 182 558 652 55(4)
1.4	-0.630 310 459 796 666(2)	5.0	-0.612 126 901 612 03(2)
1.5	-0.642 119 737 089 215(4)	5.1	-0.612 145 722 764 21(4)
1.6	-0.650 225 634 282 811(7)	5.2	-0.612 229 820 216 67(4)
1.7	-0.655 501 642 316 257(4)	5.3	-0.612 370 880 444 63(5)
1.8	-0.658 611 819 722 805(8)	5.4	-0.612 561 413 542 328(6)
1.9	-0.660 107 400 109 173(9)	5.5	-0.612 794 665 583 829(8)
2.0	-0.660 567 972 914 286(8)	5.6	-0.613 064 525 058 694(6)
2.1	-0.660 250 897 704 916(6)	5.7	-0.613 365 435 474 786(5)
2.2	-0.659 216 201 994 195(7)	5.8	-0.613 692 321 260 887(5)
2.3	-0.657 609 692 818 079(6)	5.9	-0.614 040 529 789 983(5)
2.4	-0.655 570 311 845 531(6)	6.0	-0.614 405 789 105 24(5)
2.5	-0.653 213 942 901 49(5)	6.5	-0.616 362 022 343 828(2)
2.6	-0.650 635 527 091 49(2)	7.0	-0.618 289 575 924 0(8)
2.7	-0.647 912 848 890 68(2)	7.5	-0.619 987 091 921 9(7)
2.8	-0.645 109 902 827 123(9)	8.0	-0.621 378 508 143 8(3)
2.9	-0.642 279 614 139 089(9)	8.5	-0.622 462 388 975 01(2)
3.0	-0.639 465 977 332 637(7)	9.0	-0.623 273 454 286 6(1)
3.1	-0.636 705 712 167 67(2)	9.5	-0.623 859 300 977 7(5)
3.2	-0.634 029 525 009 03(2)	10.0	-0.624 268 327 453 19(3)
3.3	-0.631 463 046 232 689(8)	11.0	-0.624 724 496 873 96(3)
3.4	-0.629 027 500 845 529(8)	12.0	-0.624 909 228 002 35(2)
3.5	-0.626 740 161 589 626(9)	13.0	-0.624 977 636 045 535(4)
3.6	-0.624 614 631 336 522(9)	14.0	-0.625 001 000 657 470(4)
3.7	-0.622 661 003 214 33(2)	15.0	-0.625 007 604 725 696(2)
3.8	-0.620 885 950 355 70(2)	16.0	-0.625 008 244 306 664(2)
3.9	-0.619 292 799 314 85(3)	17.0	-0.625 007 034 396 362 1(2)
4.0	-0.617 881 638 806 69(2)	18.0	-0.625 005 498 542 942 8(3)
4.1	-0.616 649 506 095 52(2)	19.0	-0.625 004 140 942 777 5(3)
4.2	-0.615 590 676 766 45(2)	20.0	-0.625 003 075 431 600 2(2)

Table S9: Calculated BO energies of the $3^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$3^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.238 502 584 901 1(5)	4.3	-0.589 777 941 367 421 9(2)
0.8	-0.360 428 580 812 6(3)	4.4	-0.587 397 930 925 423 8(4)
0.9	-0.446 299 293 025 778(8)	4.5	-0.585 147 011 234 322 6(3)
1.0	-0.507 905 409 337 34(3)	4.6	-0.583 024 545 273 709 1(2)
1.1	-0.552 631 673 439 913(6)	4.7	-0.581 029 432 141 636 3(2)
1.2	-0.585 305 949 989 59(2)	4.8	-0.579 160 144 174 822 4(2)
1.3	-0.609 195 081 549 09(2)	4.9	-0.577 414 748 191 591 3(2)
1.4	-0.626 572 901 213 61(2)	5.0	-0.575 790 910 544 798 9(4)
1.5	-0.639 059 645 911 36(2)	5.1	-0.574 285 885 014 758 4(6)
1.6	-0.647 832 562 245 35(2)	5.2	-0.572 896 482 352 946 7(9)
1.7	-0.653 760 067 134 403(9)	5.3	-0.571 619 021 058 419(2)
1.8	-0.657 485 408 507 765(4)	5.4	-0.570 449 261 522 866(2)
1.9	-0.659 451 216 919 32 1(4)	5.5	-0.569 382 330 811 155(2)
2.0	-0.659 842 081 203 761(2)	5.6	-0.568 412 653 201 142(3)
2.1	-0.658 994 131 399 812(4)	5.7	-0.567 533 910 643 625(3)
2.2	-0.657 312 396 926 138(3)	5.8	-0.566 739 063 418 33(2)
2.3	-0.655 018 414 880 138(3)	5.9	-0.566 020 458 486 05(2)
2.4	-0.652 265 508 883 909(2)	6.0	-0.565 370 036 969 41(2)
2.5	-0.649 171 859 514 417 4(5)	6.5	-0.562 868 170 371 42(2)
2.6	-0.645 831 110 873 467 1(4)	7.0	-0.561 095 333 476 34(2)
2.7	-0.642 318 264 666 943 2(2)	7.5	-0.559 712 901 786 36(2)
2.8	-0.638 693 739 066 342 5(6)	8.0	-0.558 625 028 589 28(3)
2.9	-0.635 006 380 738 168 4(6)	8.5	-0.557 790 848 085 99(2)
3.0	-0.631 295 771 066 439 4(4)	9.0	-0.557 170 539 345 05(2)
3.1	-0.627 594 021 558 965 2(4)	9.5	-0.556 720 889 931 32(2)
3.2	-0.623 927 186 834 795 4(7)	10.0	-0.556 400 569 490 59(2)
3.3	-0.620 316 385 777 730(2)	11.0	-0.556 015 011 732 50(2)
3.4	-0.616 778 697 120 659(2)	12.0	-0.555 821 527 469 240(5)
3.5	-0.613 327 878 981 417 6(4)	13.0	-0.555 720 547 680 827(4)
3.6	-0.609 974 949 885 232 8(5)	14.0	-0.555 664 773 488 572(2)
3.7	-0.606 728 660 017 531 8(7)	15.0	-0.555 631 998 410 846 3(5)
3.8	-0.603 595 874 891 985 6(4)	16.0	-0.555 611 537 555 076 9(4)
3.9	-0.600 581 888 661 373 2(3)	17.0	-0.555 598 048 100 404 5(2)
4.0	-0.597 690 680 511 958 1(3)	18.0	-0.555 588 736 150 425 9(4)
4.1	-0.594 925 124 662 708 4(3)	19.0	-0.555 582 066 195 806 7(3)
4.2	-0.592 287 162 221 134 5(3)	20.0	-0.555 577 150 155 085 0(4)

Table S10: Calculated BO energies of the $4^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$4^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.217 536 646 295 9(7)	4.3	-0.577 420 960 308 37(7)
0.8	-0.339 120 034 158 1(5)	4.4	-0.575 545 117 964 44(6)
0.9	-0.424 644 979 746 7(2)	4.5	-0.573 775 776 542 70(4)
1.0	-0.485 902 620 977 2(2)	4.6	-0.572 111 684 791 37(6)
1.1	-0.530 277 685 752 4(2)	4.7	-0.570 552 232 831 47(6)
1.2	-0.562 597 748 380 5(3)	4.8	-0.569 097 537 363 06(3)
1.3	-0.586 129 236 267 3(2)	4.9	-0.567 748 442 853 43(3)
1.4	-0.603 145 612 241 14(9)	5.0	-0.566 506 405 366 9(3)
1.5	-0.615 267 089 110 14(7)	5.1	-0.565 373 200 003 48(3)
1.6	-0.623 671 993 926(2)	5.2	-0.564 350 375 533 21(3)
1.7	-0.629 233 454 598 7(3)	5.3	-0.563 438 403 824 54(3)
1.8	-0.632 614 686 635 83(9)	5.4	-0.562 635 584 491 66(3)
1.9	-0.634 361 580 666 7(2)	5.5	-0.561 936 981 619 47(4)
2.0	-0.634 921 345 054 2(2)	5.6	-0.561 333 881 960 85(4)
2.1	-0.634 517 045 186 8(2)	5.7	-0.560 814 230 915 80(4)
2.2	-0.633 339 872 893 5(2)	5.8	-0.560 364 081 294 57(3)
2.3	-0.631 565 028 867 3(2)	5.9	-0.559 969 529 406 66(3)
2.4	-0.629 336 161 586 5(4)	6.0	-0.559 618 386 261 97(2)
2.5	-0.626 769 148 397 9(3)	6.5	-0.558 265 522 045 85(2)
2.6	-0.623 957 457 965 8(2)	7.0	-0.557 356 697 113 55(2)
2.7	-0.620 976 684 328 18(8)	7.5	-0.556 771 892 089 421(9)
2.8	-0.617 888 130 508 89(7)	8.0	-0.556 402 866 207 961(5)
2.9	-0.614 741 601 243 2(3)	8.5	-0.556 165 439 419 370(5)
3.0	-0.611 577 572 735 5(2)	9.0	-0.556 007 320 666 745(2)
3.1	-0.608 428 877 219 3(4)	9.5	-0.555 898 238 881 920 2(7)
3.2	-0.605 322 010 634 0(3)	10.0	-0.555 820 619 261 740 1(3)
3.3	-0.602 278 149 299 8(3)	11.0	-0.555 721 576 607 255 2(5)
3.4	-0.599 313 945 793 2(2)	12.0	-0.555 664 356 552 250 9(7)
3.5	-0.596 442 163 556 7(2)	13.0	-0.555 629 091 958 901 9(9)
3.6	-0.593 672 201 887 8(3)	14.0	-0.555 606 300 007 258(5)
3.7	-0.591 010 555 625 9(6)	15.0	-0.555 591 101 913 952(2)
3.8	-0.588 461 245 064 0(4)	16.0	-0.555 580 778 301 408 3(2)
3.9	-0.586 026 240 310 8(6)	17.0	-0.555 573 681 918 567(2)
4.0	-0.583 705 891 023 2(3)	18.0	-0.555 568 753 593 352 7(2)
4.1	-0.581 499 359 008 28(7)	19.0	-0.555 565 293 510 907 2(3)
4.2	-0.579 405 040 595 65(7)	20.0	-0.555 562 835 328 660 0(6)

Table S11: Calculated BO energies of the $5^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$5^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.214 020 967 24(4)	4.3	-0.567 803 978 955 034(4)
0.8	-0.335 907 516 563(4)	4.4	-0.565 473 005 504 785(3)
0.9	-0.421 733 421 4735(7)	4.5	-0.563 266 868 994 272(2)
1.0	-0.483 289 150 953(2)	4.6	-0.561 188 647 017 841(3)
1.1	-0.527 959 195 692(4)	4.7	-0.559 243 775 865 617(5)
1.2	-0.560 571 136 081 5(2)	4.8	-0.557 442 655 718 874(5)
1.3	-0.584 391 505 986 6(2)	4.9	-0.555 806 110 005 774(9)
1.4	-0.601 693 821 655 83(10)	5.0	-0.554 376 501 369 61(4)
1.5	-0.614 098 033 451 2(8)	5.1	-0.553 233 215 535 24(4)
1.6	-0.622 781 220 836 5(2)	5.2	-0.552 473 692 970 09(7)
1.7	-0.628 611 939 105 16(6)	5.3	-0.552 091 713 616 97(8)
1.8	-0.632 233 939 157 06(8)	5.4	-0.551 927 991 004 74(8)
1.9	-0.634 094 715 977 20(4)	5.5	-0.551 823 343 066 11(7)
2.0	-0.634 510 600 994 14(4)	5.6	-0.551 695 218 279 26(6)
2.1	-0.633 851 198 691 45(9)	5.7	-0.551 515 129 626 29(5)
2.2	-0.632 389 351 005 35(2)	5.8	-0.551 281 423 564 62(5)
2.3	-0.630 315 951 123 95(1)	5.9	-0.551 004 137 979 47(4)
2.4	-0.627 778 113 141 50(2)	6.0	-0.550 697 173 043 07(3)
2.5	-0.624 892 241 963 812(7)	6.5	-0.549 124 852 796 01(2)
2.6	-0.621 751 364 642 482(7)	7.0	-0.547 988 911 593 2(2)
2.7	-0.618 430 248 955 305(8)	7.5	-0.547 359 463 368 8(2)
2.8	-0.614 989 220 447 405(9)	8.0	-0.547 072 839 740 56(8)
2.9	-0.611 477 083 666 765(8)	8.5	-0.546 987 588 439 29(3)
3.0	-0.607 933 389 760 105(8)	9.0	-0.547 030 416 308 4(3)
3.1	-0.604 390 214 231 849(7)	9.5	-0.547 177 967 831 11(6)
3.2	-0.600 873 561 938 394(5)	10.0	-0.547 429 975 325 12(6)
3.3	-0.597 404 485 414 363(5)	11.0	-0.548 250 619 743 45(3)
3.4	-0.593 999 981 009 364(5)	12.0	-0.549 404 819 984 75(5)
3.5	-0.590 673 711 814 572(5)	13.0	-0.550 683 731 986 42(5)
3.6	-0.587 436 595 090 516(4)	14.0	-0.551 886 873 564 60(6)
3.7	-0.584 297 283 689 725(9)	15.0	-0.552 901 828 722 30(7)
3.8	-0.581 262 565 051 711(6)	16.0	-0.553 697 959 574 33(4)
3.9	-0.578 337 697 296 83(2)	17.0	-0.554 291 614 245 07(6)
4.0	-0.575 526 699 604 009(7)	18.0	-0.554 717 881 485 92(2)
4.1	-0.572 832 613 609 267(6)	19.0	-0.555 014 750 255 88(2)
4.2	-0.570 257 754 736 699(5)	20.0	-0.555 216 042 989 90(3)

Table S12: Calculated BO energies of the $6^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$6^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.204 455 278 331(6)	4.3	-0.562 209 395 510 0(3)
0.8	-0.326 175 437 534 4(3)	4.4	-0.560 082 924 728 9(2)
0.9	-0.411 833 594 334 1(6)	4.5	-0.558 063 138 519 9(2)
1.0	-0.473 220 487 327 9(4)	4.6	-0.556 150 678 784 5(2)
1.1	-0.517 720 655 208 4(5)	4.7	-0.554 348 320 135 1(2)
1.2	-0.550 161 602 178 3(3)	4.8	-0.552 664 220 177 4(2)
1.3	-0.573 809 743 487 3(2)	4.9	-0.551 121 969 942 2(3)
1.4	-0.590 938 537 339 9(2)	5.0	-0.549 794 810 422 4(3)
1.5	-0.603 168 137 469 9(3)	5.1	-0.548 852 549 524 3(4)
1.6	-0.611 676 633 412 2(2)	5.2	-0.548 221 674 974 2(4)
1.7	-0.617 336 371 396 5(2)	5.3	-0.547 494 438 779 2(2)
1.8	-0.620 807 707 958 8(7)	5.4	-0.546 598 871 942 1(2)
1.9	-0.622 619 202 977 8(6)	5.5	-0.545 630 712 226 58(5)
2.0	-0.623 173 242 975 6(4)	5.6	-0.544 661 178 928 73(3)
2.1	-0.622 725 328 282 2(8)	5.7	-0.543 725 742 647 17(2)
2.2	-0.621 491 897 976 6(5)	5.8	-0.542 840 504 022 94(2)
2.3	-0.619 652 754 036 6(4)	5.9	-0.542 012 092 812 35(2)
2.4	-0.617 352 324 096 1(4)	6.0	-0.541 242 340 052 86(2)
2.5	-0.614 706 361 031 2(3)	6.5	-0.538 206 628 964 43(2)
2.6	-0.611 807 894 846 4(4)	7.0	-0.536 207 545 947 27(4)
2.7	-0.608 731 935 610 8(3)	7.5	-0.534 850 514 908 25(6)
2.8	-0.605 539 124 465 3(4)	8.0	-0.533 904 090 278 87(7)
2.9	-0.602 278 566 328 6(5)	8.5	-0.533 253 536 848 18(4)
3.0	-0.598 990 034 719 0(3)	9.0	-0.532 834 106 285 61(9)
3.1	-0.595 705 694 899 9(4)	9.5	-0.532 588 236 691 62(7)
3.2	-0.592 451 457 011 6(3)	10.0	-0.532 452 557 932 05(9)
3.3	-0.589 248 045 510 8(4)	11.0	-0.532 323 599 062 69(6)
3.4	-0.586 111 852 922 3(4)	12.0	-0.532 225 438 084 64(4)
3.5	-0.583 055 632 388 6(3)	13.0	-0.532 091 007 316 73(3)
3.6	-0.580 089 072 835 1(3)	14.0	-0.531 927 748 583 81(7)
3.7	-0.577 219 291 211 5(3)	15.0	-0.531 765 445 087 49(3)
3.8	-0.574 451 267 304 5(3)	16.0	-0.531 626 403 813 61(7)
3.9	-0.571 788 237 957 7(3)	17.0	-0.531 518 528 013 38(7)
4.0	-0.569 232 059 953 8(3)	18.0	-0.531 439 752 005 47(2)
4.1	-0.566 783 545 774 9(3)	19.0	-0.531 384 076 229 52(2)
4.2	-0.564 442 775 714 7(3)	20.0	-0.531 345 280 686 09(5)

Table S13: Calculated BO energies of the $7^3\Sigma_g^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$7^3\Sigma_g^+$			
R/au	E/au	R/au	E/au
0.7	-0.202 702 053 42(5)	4.3	-0.558 752 897 983 14(5)
0.8	-0.324 573 662 75(3)	4.4	-0.556 456 501 450 1(2)
0.9	-0.410 382 606 17(2)	4.5	-0.554 270 168 415 8(7)
1.0	-0.471 919 268 627(8)	4.6	-0.552 192 994 565 54(9)
1.1	-0.516 568 046 016(5)	4.7	-0.550 224 011 251 8(4)
1.2	-0.549 156 416 485(3)	4.8	-0.548 364 200 864 39(2)
1.3	-0.572 950 811 085(3)	4.9	-0.547 035 875 224(2)
1.4	-0.590 224 658 554(2)	5.0	-0.547 042 080 927(2)
1.5	-0.602 597 876 241(2)	5.1	-0.546 759 747 629 7(5)
1.6	-0.611 247 673 497 3(7)	5.2	-0.545 899 761 600 50(9)
1.7	-0.617 043 252 944 6(7)	5.3	-0.544 808 533 115 7(2)
1.8	-0.620 631 054 932 4(8)	5.4	-0.543 698 552 600 5(2)
1.9	-0.622 475 693 774(2)	5.5	-0.542 631 919 576 7(3)
2.0	-0.622 938 063 820 7(9)	5.6	-0.541 627 707 652 0(4)
2.1	-0.622 355 023 426 6(7)	5.7	-0.540 692 249 859 5(4)
2.2	-0.620 893 150 440 3(2)	5.8	-0.539 827 213 667 3(5)
2.3	-0.618 989 511 901 9(2)	5.9	-0.539 032 163 856 2(5)
2.4	-0.616 617 658 293 5(2)	6.0	-0.538 305 504 309 4(5)
2.5	-0.613 893 244 630 3(2)	6.5	-0.535 596 531 024 0(6)
2.6	-0.610 908 982 328 4(1)	7.0	-0.534 068 234 30(8)
2.7	-0.607 739 491 015 1(2)	7.5	-0.533 228 408 87(5)
2.8	-0.604 445 011 579 6(3)	8.0	-0.532 734 606 74(3)
2.9	-0.601 074 284 522(3)	8.5	-0.532 403 519 054(9)
3.0	-0.597 666 796 816(2)	9.0	-0.532 147 577 079 2(2)
3.1	-0.594 254 548 219(2)	9.5	-0.531 933 638 474 4(2)
3.2	-0.590 863 448 904(1)	10.0	-0.531 760 079 568 8(2)
3.3	-0.587 514 432 124(1)	11.0	-0.531 531 942 651 89(4)
3.4	-0.584 224 345 115(3)	12.0	-0.531 414 041 859 91(2)
3.5	-0.581 006 666 321 7(2)	13.0	-0.531 352 987 487 19(2)
3.6	-0.577 872 085 888 4(3)	14.0	-0.531 319 332 005 84(3)
3.7	-0.574 828 977 942 8(2)	15.0	-0.531 299 186 941 973(3)
3.8	-0.571 883 786 925 83(9)	16.0	-0.531 286 213 982 657(2)
3.9	-0.569 041 345 418 06(7)	17.0	-0.531 277 400 192 98(2)
4.0	-0.566 305 137 292 2(2)	18.0	-0.531 271 180 173 78(4)
4.1	-0.563 677 517 267 92(2)	19.0	-0.531 266 663 491 52(6)
4.2	-0.561 159 895 927 81(3)	20.0	-0.531 263 307 515 65(8)

Table S14: Calculated BO energies of the $1^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$1^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.342130928988667(6)	4.3	-0.653195827155049(8)
0.8	-0.46143498347982(4)	4.4	-0.65073706182336(2)
0.9	-0.544767040091894(3)	4.5	-0.6484429623517(4)
1.0	-0.60392224803181505(4)	4.6	-0.6463109963342(4)
1.1	-0.6462856755609065(2)	4.7	-0.644337697996883(3)
1.2	-0.67668314180341571(6)	4.8	-0.6425186973868(9)
1.3	-0.69837814548896884(3)	4.9	-0.64084876299434(10)
1.4	-0.7136405684873686(3)	5.0	-0.639321863500910(9)
1.5	-0.7240866205382896(3)	5.1	-0.637931252052529(10)
1.6	-0.730890086928356(5)	5.2	-0.636669573606577(10)
1.7	-0.734917974883440(1)	5.3	-0.6355289928497(10)
1.8	-0.736820091741595(7)	5.4	-0.634501337399442(10)
1.9	-0.7370896537668271(1)	5.5	-0.63357824894624(3)
2.0	-0.7361051733454439(3)	5.6	-0.6327513339942(6)
2.1	-0.7341599538590402(5)	5.7	-0.6320123060258(5)
2.2	-0.7314832061423001(5)	5.8	-0.63135311211810(10)
2.3	-0.7282553924169136(7)	5.9	-0.63076603896819(2)
2.4	-0.724619525233251(2)	6.0	-0.63024379552804(2)
2.5	-0.720689588359196(4)	6.5	-0.6283849655891246(9)
2.6	-0.716556881346118(10)	7.0	-0.627343969517241(3)
2.7	-0.712294847112937(1)	7.5	-0.6267388331983872(5)
2.8	-0.707962778269134(4)	8.0	-0.6263678024076574(9)
2.9	-0.703608685724174(4)	8.5	-0.626127410224462(2)
3.0	-0.699271535123230(2)	9.0	-0.6259640651384734(9)
3.1	-0.694983001681094(6)	9.5	-0.625848897568859(2)
3.2	-0.6907688547753517(8)	10.0	-0.625765155314512(2)
3.3	-0.6866500553689703(6)	11.0	-0.625651263865481(1)
3.4	-0.6826436287043045(9)	12.0	-0.625565960913511(5)
3.5	-0.6787633595262160(5)	13.0	-0.625485558864006(2)
3.6	-0.675020345825230(2)	14.0	-0.6254088253710753(7)
3.7	-0.6714234386847724(8)	15.0	-0.6253403831152288(4)
3.8	-0.6679795895349028(9)	16.0	-0.6252826990251769(5)
3.9	-0.66469412144608(2)	17.0	-0.62523562891080(2)
4.0	-0.661570937686215(2)	18.0	-0.6251977430164360(2)
4.1	-0.658612678362044(2)	19.0	-0.6251673111090794(2)
4.2	-0.655820834391176(3)	20.0	-0.6251427558519418(1)

Table S15: Calculated BO energies of the $2^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$2^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.238 540 424 455(2)	4.3	-0.628 854 772 172 40(9)
0.8	-0.360 658 634 698(8)	4.4	-0.628 289 641 463 10(7)
0.9	-0.446 755 626 041(9)	4.5	-0.627 830 572 168 30(7)
1.0	-0.508 623 142 870(2)	4.6	-0.627 462 667 471 31(7)
1.1	-0.553 646 688 943 9(3)	4.7	-0.627 171 731 657 94(6)
1.2	-0.586 654 492 022 5(5)	4.8	-0.626 944 690 182 90(6)
1.3	-0.610 913 265 794 4(4)	4.9	-0.626 769 837 544 22(5)
1.4	-0.628 696 166 670 8(3)	5.0	-0.626 636 941 335 93(5)
1.5	-0.641 622 261 629 4(3)	5.1	-0.626 537 237 798 72(5)
1.6	-0.650 867 490 300 8(4)	5.2	-0.626 463 353 422 52(4)
1.7	-0.657 300 177 092 73(9)	5.3	-0.626 409 182 048 89(4)
1.8	-0.661 570 604 624 8(2)	5.4	-0.626 369 740 200(4)
1.9	-0.664 171 730 539 8(9)	5.5	-0.626 341 016 761 7(2)
2.0	-0.665 481 275 550 3(2)	5.6	-0.626 319 827 566(3)
2.1	-0.665 791 485 720 9(4)	5.7	-0.626 303 681 077(3)
2.2	-0.665 330 550 891 5(3)	5.8	-0.626 290 658 314(3)
2.3	-0.664 278 251 340 4(2)	5.9	-0.626 279 308 035(2)
2.4	-0.662 777 529 478 7(3)	6.0	-0.626 268 556 926(2)
2.5	-0.660 943 130 019 5(9)	6.5	-0.626 204 120 508 69(6)
2.6	-0.658 868 095 962 8(7)	7.0	-0.626 108 840 692 92(4)
2.7	-0.656 628 673 762 7(6)	7.5	-0.625 992 825 518 12(3)
2.8	-0.654 288 023 140 9(7)	8.0	-0.625 871 959 125 05(7)
2.9	-0.651 899 016 987 6(6)	8.5	-0.625 757 136 296 18(4)
3.0	-0.649 506 337 701 2(6)	9.0	-0.625 653 723 782 34(2)
3.1	-0.647 148 018 363 9(6)	9.5	-0.625 563 326 779 57(2)
3.2	-0.644 856 535 091 5(9)	10.0	-0.625 485 476 179 07(2)
3.3	-0.642 659 528 387 4(4)	11.0	-0.625 361 446 815 16(2)
3.4	-0.640 580 215 713 0(3)	12.0	-0.625 268 383 823 90(2)
3.5	-0.638 637 554 497 7(3)	13.0	-0.625 194 812 171 22(2)
3.6	-0.636 846 223 249 7(2)	14.0	-0.625 133 338 171 65(3)
3.7	-0.635 216 504 171 0(2)	15.0	-0.625 082 653 714 59(6)
3.8	-0.633 754 166 066 6(2)	16.0	-0.625 046 272 685 48(6)
3.9	-0.632 460 450 830 4(2)	17.0	-0.625 024 588 810 57(2)
4.0	-0.631 332 251 015 4(2)	18.0	-0.625 013 158 472 31(2)
4.1	-0.630 362 527 158 92(9)	19.0	-0.625 007 381 376 735(9)
4.2	-0.629 540 959 158 75(9)	20.0	-0.625 004 422 300 836(8)

Table S16: Calculated BO energies of the $3^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$3^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.214 021 007 253(4)	4.3	-0.584 590 871 106 42
0.8	-0.335 988 249 501(4)	4.4	-0.582 905 438 381 35
0.9	-0.421 909 252 39(3)	4.5	-0.581 291 512 643 71
1.0	-0.483 574 887 235(4)	4.6	-0.579 743 429 521 85
1.1	-0.528 369 903 241(3)	4.7	-0.578 257 136 745 01
1.2	-0.561 121 954 872(3)	4.8	-0.576 830 034 039 14
1.3	-0.585 097 432 476(2)	4.9	-0.575 460 751 291 77
1.4	-0.602 569 486 863(4)	5.0	-0.574 148 957 152 82
1.5	-0.615 157 555 458(2)	5.1	-0.572 895 298 055 85
1.6	-0.624 038 363 274 6(7)	5.2	-0.571 701 640 995 6(
1.7	-0.630 081 444 707 3(5)	5.3	-0.570 572 093 118 0(
1.8	-0.633 938 689 449 4(8)	5.4	-0.569 516 528 945 2(
1.9	-0.636 104 990 662 4(7)	5.5	-0.568 565 001 336 4(
2.0	-0.636 960 224 981 2(7)	5.6	-0.567 847 815 180 2(
2.1	-0.636 798 875 149 4(6)	5.7	-0.567 886 332 107 2(
2.2	-0.635 851 290 216 6(6)	5.8	-0.568 770 542 884 0(
2.3	-0.634 299 171 228 4(6)	5.9	-0.569 907 886 493 0(
2.4	-0.632 286 995 016 4(6)	6.0	-0.571 113 781 545 9(
2.5	-0.629 930 532 534(2)	6.5	-0.577 231 863 256 4(
2.6	-0.627 323 257 529 3(6)	7.0	-0.583 002 416 789 2(
2.7	-0.624 541 202 247(2)	7.5	-0.588 215 781 977 0(
2.8	-0.621 646 654 410 3(9)	8.0	-0.592 774 998 348 6(
2.9	-0.618 690 976 162(4)	8.5	-0.596 634 758 932 7(
3.0	-0.615 716 744 253 4(3)	9.0	-0.599 788 095 817 9(
3.1	-0.612 759 351 372 8(3)	9.5	-0.602 249 087 682 8(
3.2	-0.609 848 165 915(1)	10.0	-0.604 036 751 120 6
3.3	-0.607 007 319 761 8(7)	11.0	-0.605 646 762 091 9
3.4	-0.604 256 182 175 3(9)	12.0	-0.604 785 946 817(2)
3.5	-0.601 609 583 431 3(8)	13.0	-0.602 054 108 577 6
3.6	-0.599 077 875 434 9(3)	14.0	-0.598 400 117 003(2)
3.7	-0.596 666 949 461 9(4)	15.0	-0.594 530 173 646(8)
3.8	-0.594 378 356 240 0(2)	16.0	-0.590 782 328 490(3)
3.9	-0.592 209 665 274 5(5)	17.0	-0.587 283 406 929(9)
4.0	-0.590 155 140 819 4(2)	18.0	-0.584 067 028 544(6)
4.1	-0.588 206 709 198 15(5)	19.0	-0.581 128 783 061(5)
4.2	-0.586 355 085 847 83(3)	20.0	-0.578 449 723 123(8)

Table S17: Calculated BO energies of the $4^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$4^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.213 906 164 232 6(4)	4.3	-0.571 691 450 940 6(3)
0.8	-0.335 769 148 880 7(4)	4.4	-0.569 647 202 397 9(2)
0.9	-0.421 568 270 896 8(8)	4.5	-0.567 776 268 871 9(3)
1.0	-0.483 093 840 186 66(4)	4.6	-0.566 101 351 451 7(4)
1.1	-0.527 730 172 074 9(2)	4.7	-0.564 654 775 476 3(7)
1.2	-0.560 304 664 538 7(4)	4.8	-0.563 480 505 873 2(2)
1.3	-0.584 083 680 981 18(6)	4.9	-0.562 631 618 145 3(2)
1.4	-0.601 340 622 656 0(2)	5.0	-0.562 157 285 797 7(3)
1.5	-0.613 695 490 244 74(2)	5.1	-0.562 078 705 044 2(4)
1.6	-0.622 325 899 136 6(2)	5.2	-0.562 369 841 571 5(5)
1.7	-0.628 102 586 324 313(6)	5.3	-0.562 962 553 827 7(6)
1.8	-0.631 678 906 894 82(2)	5.4	-0.563 768 473 968 7(3)
1.9	-0.633 551 397 356 628(6)	5.5	-0.564 686 467 426 1(3)
2.0	-0.634 101 640 058 24(1)	5.6	-0.565 531 127 724 5(2)
2.1	-0.633 625 749 505 14(1)	5.7	-0.565 741 533 935 86(6)
2.2	-0.632 355 489 126 19(2)	5.8	-0.565 200 181 631 13(2)
2.3	-0.630 473 621 015 76(2)	5.9	-0.564 480 599 566 02(2)
2.4	-0.628 125 214 112 91(3)	6.0	-0.563 754 048 912 11(4)
2.5	-0.625 426 076 547 48(2)	6.5	-0.560 690 481 657 35(9)
2.6	-0.622 469 113 267 93(2)	7.0	-0.558 660 645 296 63(9)
2.7	-0.619 329 168 109 14(3)	7.5	-0.557 439 918 687 02(8)
2.8	-0.616 066 746 179 73(2)	8.0	-0.556 748 255 724 83(6)
2.9	-0.612 730 900 574 67(2)	8.5	-0.556 360 513 516 78(6)
3.0	-0.609 361 489 708 66(2)	9.0	-0.556 135 526 415 02(5)
3.1	-0.605 990 956 927 08(2)	9.5	-0.555 996 879 725 81(3)
3.2	-0.602 645 745 239 60(2)	10.0	-0.555 905 557 053 50(2)
3.3	-0.599 347 432 246 56(2)	11.0	-0.555 793 967 498 227(8)
3.4	-0.596 113 650 396 64(3)	12.0	-0.555 726 877 530 804(6)
3.5	-0.592 958 843 506 38(2)	13.0	-0.555 681 048 545 983(4)
3.6	-0.589 894 900 612 93(2)	14.0	-0.555 648 509 857 390(6)
3.7	-0.586 931 701 910 95(2)	15.0	-0.555 625 337 538 939(2)
3.8	-0.584 077 608 409 18(3)	16.0	-0.555 608 805 601 579(5)
3.9	-0.581 339 927 183 06(3)	17.0	-0.555 596 911 087 659(6)
4.0	-0.578 725 388 419 23(7)	18.0	-0.555 588 233 968 701(3)
4.1	-0.576 240 680 300 24(9)	19.0	-0.555 581 798 259 419(2)
4.2	-0.573 893 105 460 8(2)	20.0	-0.555 576 941 975 60(2)

Table S18: Calculated BO energies of the $5^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$5^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.202 698 747 624(7)	4.3	-0.566 204 349 790(2)
0.8	-0.324 611 637 060(9)	4.4	-0.564 235 019 697 9(5)
0.9	-0.410 469 233 105(9)	4.5	-0.562 363 520 035 3(6)
1.0	-0.472 062 106 988(7)	4.6	-0.560 591 206 703 2(10)
1.1	-0.516 774 760 61(4)	4.7	-0.558 921 660 050(2)
1.2	-0.549 434 677 53(2)	4.8	-0.557 361 064 460 6(9)
1.3	-0.573 308 178 74(2)	4.9	-0.555 918 540 232(2)
1.4	-0.590 668 470 95(2)	5.0	-0.554 606 051 944(2)
1.5	-0.603 135 191 497(9)	5.1	-0.553 437 400 176(2)
1.6	-0.611 885 418 804(3)	5.2	-0.552 426 762 276(3)
1.7	-0.617 789 190 774(3)	5.3	-0.551 588 911 394(3)
1.8	-0.621 499 031 411(2)	5.4	-0.550 940 811 352(2)
1.9	-0.623 510 562 954(2)	5.5	-0.550 497 606 148(2)
2.0	-0.624 204 434 706(6)	5.6	-0.550 259 504 182(2)
2.1	-0.623 875 883 460(2)	5.7	-0.550 202 087 571(2)
2.2	-0.622 755 926 597(2)	5.8	-0.550 283 188 237 1(7)
2.3	-0.621 026 782 50(3)	5.9	-0.550 458 541 469 0(6)
2.4	-0.618 833 237 390(2)	6.0	-0.550 691 957 933 5(5)
2.5	-0.616 291 119 942(2)	6.5	-0.552 071 964 380 8(2)
2.6	-0.613 493 682 603(2)	7.0	-0.553 241 483 751 47(8)
2.7	-0.610 516 447 970(2)	7.5	-0.554 089 771 334 08(7)
2.8	-0.607 420 915 206(2)	8.0	-0.554 676 025 948 38(6)
2.9	-0.604 257 408 058(2)	8.5	-0.555 066 171 842 47(4)
3.0	-0.601 067 265 331(2)	9.0	-0.555 314 884 899 87(3)
3.1	-0.597 884 516 311(6)	9.5	-0.555 465 446 601 27(3)
3.2	-0.594 737 141 533(2)	10.0	-0.555 550 768 354 28(2)
3.3	-0.591 647 990 785(1)	11.0	-0.555 613 982 634 26(2)
3.4	-0.588 635 415 77(6)	12.0	-0.555 617 638 054 840(4)
3.5	-0.585 713 675 572(3)	13.0	-0.555 606 591 245 903(2)
3.6	-0.582 893 189 761(3)	14.0	-0.555 594 581 646 624(7)
3.7	-0.580 180 740 449(2)	15.0	-0.555 584 723 664 535 2(5)
3.8	-0.577 579 744 019(2)	16.0	-0.555 577 234 487 855 9(2)
3.9	-0.575 090 701 718 6(7)	17.0	-0.555 571 693 255 464 18(3)
4.0	-0.572 711 879 501 1(4)	18.0	-0.555 567 628 207 418 56(3)
4.1	-0.570 440 174 549 69(3)	19.0	-0.555 564 648 719 308 1(2)
4.2	-0.568 272 044 114 9(4)	20.0	-0.555 562 458 311 051 89(3)

Table S19: Calculated BO energies of the $6^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$6^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.202 641 543 808(4)	4.3	-0.559 677 367 918(9)
0.8	-0.324 500 857 535(2)	4.4	-0.557 572 619 296(1)
0.9	-0.410 295 833 993(2)	4.5	-0.555 648 421 851(2)
1.0	-0.471 816 777 429 8(2)	4.6	-0.553 939 738 997(3)
1.1	-0.516 447 995 872 22(3)	4.7	-0.552 494 223 188(5)
1.2	-0.549 016 878 249 94(1)	4.8	-0.551 354 534 192(2)
1.3	-0.572 789 776 992 8(2)	4.9	-0.550 509 617 707(2)
1.4	-0.590 040 080 229 1(2)	5.0	-0.549 858 443 017(2)
1.5	-0.602 387 773 084 99(8)	5.1	-0.549 258 749 173(2)
1.6	-0.611 010 452 631 0(2)	5.2	-0.548 614 881 226(2)
1.7	-0.616 778 834 388 37(4)	5.3	-0.547 908 676 997(2)
1.8	-0.620 346 248 365 47(4)	5.4	-0.547 171 579 357(1)
1.9	-0.622 209 201 857 97(2)	5.5	-0.546 445 037 727(1)
2.0	-0.622 749 243 256 95(3)	5.6	-0.545 755 698 385(1)
2.1	-0.622 262 447 660 2(2)	5.7	-0.545 111 046 755(1)
2.2	-0.620 980 532 821 3(1)	5.8	-0.544 510 214 674(5)
2.3	-0.619 086 207 950 0(2)	5.9	-0.543 954 125 096(5)
2.4	-0.616 724 480 797 8(1)	6.0	-0.543 447 051 824(6)
2.5	-0.614 011 088 742 4(1)	6.5	-0.541 776 292 713(6)
2.6	-0.611 038 854 955 7(1)	7.0	-0.541 331 654 425(6)
2.7	-0.607 882 528 785 2(2)	7.5	-0.541 289 909 323(4)
2.8	-0.604 602 506 195 7(2)	8.0	-0.541 181 860 253(4)
2.9	-0.601 247 714 248 1(2)	8.5	-0.540 972 160 924(2)
3.0	-0.597 857 865 881 8(3)	9.0	-0.540 737 779 255(2)
3.1	-0.594 465 236 648 7(2)	9.5	-0.540 546 319 996(2)
3.2	-0.591 096 076 267 1(2)	10.0	-0.540 441 347 155(2)
3.3	-0.587 771 740 160 8(2)	11.0	-0.540 590 594 603(2)
3.4	-0.584 509 606 364 2(2)	12.0	-0.541 303 924 753(2)
3.5	-0.581 323 829 246 2(2)	13.0	-0.542 575 402 077(2)
3.6	-0.578 225 972 200 3(3)	14.0	-0.544 253 876 152(3)
3.7	-0.575 225 556 202 0(5)	15.0	-0.546 098 788 249(3)
3.8	-0.572 330 560 132 6(5)	16.0	-0.547 891 392 065(2)
3.9	-0.569 547 913 186 9(8)	17.0	-0.549 495 899 070(5)
4.0	-0.566 884 032 335(4)	18.0	-0.550 855 689 336(3)
4.1	-0.564 345 484 236(4)	19.0	-0.551 965 794 737(5)
4.2	-0.561 939 901 191(6)	20.0	-0.552 848 073 525(2)

Table S20: Calculated BO energies of the $7^1\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$7^1\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.196 556 267 4(4)	4.3	-0.556 938 194 00(3)
0.8	-0.318 444 971 68(4)	4.4	-0.554 868 900 09(5)
0.9	-0.404 274 355 18(4)	4.5	-0.552 924 316 40(7)
1.0	-0.465 834 863 6(1)	4.6	-0.551 116 724 31(9)
1.1	-0.510 510 900 51(4)	4.7	-0.549 464 235 12(9)
1.2	-0.543 129 888 44(3)	4.8	-0.547 989 623 6(2)
1.3	-0.566 958 136 56(4)	4.9	-0.546 718 181 0(2)
1.4	-0.584 268 898 86(5)	5.0	-0.545 680 081 84(10)
1.5	-0.596 681 926 67(2)	5.1	-0.544 904 994 51(9)
1.6	-0.605 374 482 19(6)	5.2	-0.544 384 430 98(7)
1.7	-0.611 216 852 95(5)	5.3	-0.544 039 377 82(4)
1.8	-0.614 861 867 57(6)	5.4	-0.543 748 047 48(4)
1.9	-0.616 805 488 67(5)	5.5	-0.543 401 862 91(2)
2.0	-0.617 428 715 95(6)	5.6	-0.542 943 778 177(4)
2.1	-0.617 027 115 96(3)	5.7	-0.542 374 970 044 8(6)
2.2	-0.615 831 983 44(6)	5.8	-0.541 730 622 372(4)
2.3	-0.614 025 730 97(6)	5.9	-0.541 050 202 482(7)
2.4	-0.611 753 229 87(4)	6.0	-0.540 363 586 475(10)
2.5	-0.609 130 265 30(3)	6.5	-0.537 295 739 035 2(6)
2.6	-0.606 249 905 64(3)	7.0	-0.535 112 105 520 7(2)
2.7	-0.603 187 345 35(3)	7.5	-0.533 708 015 890 9(4)
2.8	-0.600 003 616 43(6)	8.0	-0.532 851 179 857(3)
2.9	-0.596 748 451 37(6)	8.5	-0.532 337 574 887(2)
3.0	-0.593 462 499 75(5)	9.0	-0.532 029 019 452 9(8)
3.1	-0.590 179 044 58(5)	9.5	-0.531 842 386 687 8(3)
3.2	-0.586 925 322 06(4)	10.0	-0.531 729 266 581 1(3)
3.3	-0.583 723 520 71(10)	11.0	-0.531 614 010 327 5(2)
3.4	-0.580 591 518 63(8)	12.0	-0.531 549 113 952 7(2)
3.5	-0.577 543 413 32(4)	13.0	-0.531 494 826 517 9(2)
3.6	-0.574 589 908 10(5)	14.0	-0.531 446 915 404 6(9)
3.7	-0.571 738 636 58(2)	15.0	-0.531 406 369 096(3)
3.8	-0.568 994 520 991(6)	16.0	-0.531 373 303 038(3)
3.9	-0.566 360 254 44(1)	17.0	-0.531 346 928 831(4)
4.0	-0.563 836 955 134(5)	18.0	-0.531 326 139 881(5)
4.1	-0.561 424 980 109(7)	19.0	-0.531 309 849 441(5)
4.2	-0.559 124 842 78(2)	20.0	-0.531 297 117 483 24(4)

Table S21: Calculated BO energies of the $2^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$2^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.245 149 517 334 5(2)	4.3	-0.632 300 341 455 545(2)
0.8	-0.368 332 096 096 89(4)	4.4	-0.630 946 270 507 275(2)
0.9	-0.455 605 952 653 3(2)	4.5	-0.629 752 332 465 679(3)
1.0	-0.518 727 298 884 55(2)	4.6	-0.628 711 272 602 945(2)
1.1	-0.565 032 494 492 68(4)	4.7	-0.627 813 848 138 214(2)
1.2	-0.599 293 589 547 7(1)	4.8	-0.627 049 230 707 203(2)
1.3	-0.624 723 079 547 7(8)	4.9	-0.626 405 485 630 473(2)
1.4	-0.643 549 854 833 49(8)	5.0	-0.625 870 080 464 611(2)
1.5	-0.657 363 112 434 248(5)	5.1	-0.625 430 373 331 476(2)
1.6	-0.667 323 788 202 58(2)	5.2	-0.625 074 039 719 545(2)
1.7	-0.674 297 785 403 265(10)	5.3	-0.624 789 411 056 880(2)
1.8	-0.678 942 138 555 728(9)	5.4	-0.624 565 714 566 977(2)
1.9	-0.681 762 379 011 0(2)	5.5	-0.624 393 217 796 996(2)
2.0	-0.683 151 888 034 877(5)	5.6	-0.624 263 290 644 980(2)
2.1	-0.683 419 654 413 064(9)	5.7	-0.624 168 402 402 467(2)
2.2	-0.682 810 323 097 895(5)	5.8	-0.624 102 072 144 993(1)
2.3	-0.681 518 956 969 674(7)	5.9	-0.624 058 789 076 94(2)
2.4	-0.679 702 073 874 316(4)	6.0	-0.624 033 916 433 984(2)
2.5	-0.677 486 001 519 539(6)	6.5	-0.624 071 951 793 777(2)
2.6	-0.674 973 267 207 350(2)	7.0	-0.624 211 780 405 681(2)
2.7	-0.672 247 527 546 03(3)	7.5	-0.624 355 079 362 741(9)
2.8	-0.669 377 400 742 445(3)	8.0	-0.624 477 359 273 812(4)
2.9	-0.666 419 465 423 273(3)	8.5	-0.624 577 609 803 405(4)
3.0	-0.663 420 620 078 305(4)	9.0	-0.624 660 416 828 66(6)
3.1	-0.660 419 946 811 376(4)	9.5	-0.624 730 386 530 455(3)
3.2	-0.657 450 186 116 804(3)	10.0	-0.624 790 760 536 301 7(8)
3.3	-0.654 538 901 907 307(3)	11.0	-0.624 888 518 903 934(3)
3.4	-0.651 709 395 361 588(3)	12.0	-0.624 956 163 048 346 6(9)
3.5	-0.648 981 410 606 303(3)	13.0	-0.624 994 023 194 899(2)
3.6	-0.646 371 663 739 601(4)	14.0	-0.625 009 826 714 532(2)
3.7	-0.643 894 218 703 247(2)	15.0	-0.625 013 668 270 148 81(7)
3.8	-0.641 560 728 869 722(3)	16.0	-0.625 012 574 523 467 6(6)
3.9	-0.639 380 562 008 245(2)	17.0	-0.625 010 092 166 630 3(4)
4.0	-0.637 360 828 579 427(2)	18.0	-0.625 007 644 154 596 8(2)
4.1	-0.635 506 338 738 168(3)	19.0	-0.625 005 654 518 146 4(3)
4.2	-0.633 819 520 844 898(3)	20.0	-0.625 004 157 153 325 36(2)

Table S22: Calculated BO energies of the $3^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$3^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.216 737 782 218(7)	4.3	-0.583 343 745 660 32(2)
0.8	-0.339 106 607 001(8)	4.4	-0.581 570 068 610 58(2)
0.9	-0.425 460 109 053(8)	4.5	-0.580 015 682 532 28(2)
1.0	-0.487 572 969 892 3(2)	4.6	-0.578 731 807 044 21(2)
1.1	-0.532 810 065 278 4(4)	4.7	-0.577 827 919 057 791(10)
1.2	-0.565 978 385 627 6(3)	4.8	-0.577 514 960 007 280(8)
1.3	-0.590 326 047 186 7(5)	4.9	-0.578 005 698 878 75(3)
1.4	-0.608 112 632 892 9(2)	5.0	-0.579 213 401 148 5(2)
1.5	-0.620 949 595 684 97(5)	5.1	-0.580 844 205 472 56(8)
1.6	-0.630 010 861 558 16(5)	5.2	-0.582 680 066 704 3(2)
1.7	-0.636 167 234 930 92(3)	5.3	-0.584 604 215 739 3(2)
1.8	-0.640 074 645 883 66(4)	5.4	-0.586 553 664 245 22(3)
1.9	-0.642 233 639 427 51(4)	5.5	-0.588 491 556 144 66(3)
2.0	-0.643 030 453 676 4(2)	5.6	-0.590 394 826 357 39(4)
2.1	-0.642 765 995 260 70(7)	5.7	-0.592 248 487 712 10(4)
2.2	-0.641 676 659 330 86(9)	5.8	-0.594 042 703 935 80(2)
2.3	-0.639 949 530 353 8(4)	5.9	-0.595 771 126 422 99(2)
2.4	-0.637 733 635 167 21(2)	6.0	-0.597 429 864 492 095(10)
2.5	-0.635 148 375 657 781(8)	6.5	-0.604 643 583 377 05(2)
2.6	-0.632 289 917 107 85(8)	7.0	-0.610 164 283 471 734(2)
2.7	-0.629 236 076 002 63(2)	7.5	-0.614 274 655 129 412(5)
2.8	-0.626 050 094 269 150(4)	8.0	-0.617 281 722 559 672(7)
2.9	-0.622 783 579 123 9(2)	8.5	-0.619 453 749 372 869(7)
3.0	-0.619 478 812 428 38(2)	9.0	-0.621 006 626 945 171(5)
3.1	-0.616 170 580 166 219(2)	9.5	-0.622 107 040 260 207(5)
3.2	-0.612 887 634 475 419(2)	10.0	-0.622 880 687 353 616(3)
3.3	-0.609 653 873 013 346(4)	11.0	-0.623 797 094 063 254(2)
3.4	-0.606 489 300 197 90(3)	12.0	-0.624 243 509 019 487 7(10)
3.5	-0.603 410 819 936 905 5(8)	13.0	-0.624 472 314 386 112 5(6)
3.6	-0.600 432 898 426 203 4(7)	14.0	-0.624 602 184 111 303 9(4)
3.7	-0.597 568 127 662 870 7(9)	15.0	-0.624 684 597 977 336 3(2)
3.8	-0.594 827 715 430 413 2(4)	16.0	-0.624 741 916 484 990 00(10)
3.9	-0.592 221 926 945 15(2)	17.0	-0.624 784 492 239 311 43(6)
4.0	-0.589 760 511 276 83(2)	18.0	-0.624 817 546 382 250 07(4)
4.1	-0.587 453 173 067 53(2)	19.0	-0.624 843 960 802 916 82(2)
4.2	-0.585 310 224 662 25(2)	20.0	-0.624 865 475 830 592 93(6)

Table S23: Calculated BO energies of the $4^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$4^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.213 906 229 898 5(4)	4.3	-0.571 961 453 137 25(2)
0.8	-0.335 769 226 266 6(3)	4.4	-0.570 256 295 832 041(5)
0.9	-0.421 568 361 683 52(6)	4.5	-0.569 255 219 981 32(2)
1.0	-0.483 093 946 080 72(9)	4.6	-0.569 318 920 199 38(3)
1.1	-0.527 730 294 814 35(9)	4.7	-0.570 052 220 598 22(5)
1.2	-0.560 304 805 869 79(6)	4.8	-0.570 759 342 615 79(7)
1.3	-0.584 083 842 621 311(5)	4.9	-0.570 987 809 442 78(8)
1.4	-0.601 340 806 245 561(6)	5.0	-0.570 710 262 697 54(8)
1.5	-0.613 695 697 286 332(3)	5.1	-0.570 150 554 402 59(9)
1.6	-0.622 326 130 920 61(4)	5.2	-0.569 475 414 455 87(9)
1.7	-0.628 102 843 840 50(5)	5.3	-0.568 761 667 461 58(9)
1.8	-0.631 679 190 729 689(8)	5.4	-0.568 041 298 749 73(2)
1.9	-0.633 551 707 577 880(4)	5.5	-0.567 327 752 612 42(2)
2.0	-0.634 101 976 090 493(4)	5.6	-0.566 627 056 431 23(2)
2.1	-0.633 626 110 005 135(10)	5.7	-0.565 942 333 899 12(2)
2.2	-0.632 355 871 872 489(5)	5.8	-0.565 275 616 802 70(2)
2.3	-0.630 474 022 839 470(7)	5.9	-0.564 628 541 191 54(2)
2.4	-0.628 125 630 913 351(5)	6.0	-0.564 002 582 901 11(3)
2.5	-0.625 426 503 465 334(6)	6.5	-0.561 232 760 606 4(2)
2.6	-0.622 469 545 133 671(4)	7.0	-0.559 130 159 228 80(2)
2.7	-0.619 329 600 357 573(6)	7.5	-0.557 691 330 477 83(2)
2.8	-0.616 067 176 539 832(2)	8.0	-0.556 806 412 187 93(2)
2.9	-0.612 731 332 038 507(2)	8.5	-0.556 310 383 644 16(3)
3.0	-0.609 361 935 607 286(4)	9.0	-0.556 052 033 262 45(2)
3.1	-0.605 991 449 491 318(4)	9.5	-0.555 923 121 618 97(2)
3.2	-0.602 646 349 976 706(3)	10.0	-0.555 852 134 732 682(10)
3.3	-0.599 348 272 155 293(3)	11.0	-0.555 761 041 228 978(6)
3.4	-0.596 114 947 132 426(2)	12.0	-0.555 695 256 979 466(4)
3.5	-0.592 960 988 433 888(6)	13.0	-0.555 648 716 718 361(3)
3.6	-0.589 898 580 089 736(5)	14.0	-0.555 617 551 323 114(9)
3.7	-0.586 938 124 473 674(2)	15.0	-0.555 597 235 558 680(3)
3.8	-0.584 088 931 750 49(2)	16.0	-0.555 584 055 390 848 9(5)
3.9	-0.581 360 097 730 429(3)	17.0	-0.555 575 429 534 386(2)
4.0	-0.578 761 889 481 352(4)	18.0	-0.555 569 693 371 038 5(8)
4.1	-0.576 308 447 892 993(5)	19.0	-0.555 565 805 258 601 3(2)
4.2	-0.574 024 159 276 663(8)	20.0	-0.555 563 117 244 983 3(3)

Table S24: Calculated BO energies of the $5^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$5^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.204 068 665 129(4)	4.3	-0.565 957 163 030 17(3)
0.8	-0.326 175 387 839(2)	4.4	-0.564 959 311 005 42(6)
0.9	-0.412 239 095 498(4)	4.5	-0.564 486 638 900 60(5)
1.0	-0.474 042 043 214(7)	4.6	-0.563 696 078 158 71(3)
1.1	-0.518 958 982 599(5)	4.7	-0.562 470 949 532 53(3)
1.2	-0.551 807 651 512(5)	4.8	-0.561 123 149 558 22(5)
1.3	-0.575 846 083 804(1)	4.9	-0.559 815 017 500 65(6)
1.4	-0.593 341 620 396(1)	5.0	-0.558 612 255 490 86(9)
1.5	-0.605 910 726 312(3)	5.1	-0.557 544 903 452 0(2)
1.6	-0.614 729 712 369(3)	5.2	-0.556 626 886 870 6(2)
1.7	-0.620 669 677 920 6(5)	5.3	-0.555 861 556 982 6(2)
1.8	-0.624 385 413 810 4(4)	5.4	-0.555 243 827 519 3(3)
1.9	-0.626 375 475 030 8(6)	5.5	-0.554 762 330 629 2(3)
2.0	-0.627 023 695 869 2(3)	5.6	-0.554 401 945 352 3(3)
2.1	-0.626 628 454 964 4(3)	5.7	-0.554 146 020 110 1(4)
2.2	-0.625 423 667 380 3(2)	5.8	-0.553 977 896 274 2(4)
2.3	-0.623 594 074 924 95(5)	5.9	-0.553 881 821 343 7(4)
2.4	-0.621 286 535 592 08(10)	6.0	-0.553 843 471 799 9(4)
2.5	-0.618 618 460 850 74(6)	6.5	-0.554 137 549 477 94(4)
2.6	-0.615 684 191 079 4(2)	7.0	-0.554 661 498 483 50(3)
2.7	-0.612 559 861 941 78(4)	7.5	-0.555 095 897 556 77(2)
2.8	-0.609 307 154 255 60(3)	8.0	-0.555 383 467 526 39(2)
2.9	-0.605 976 210 065 99(6)	8.5	-0.555 542 697 349 489(5)
3.0	-0.602 607 921 428 56(5)	9.0	-0.555 606 991 057 5(3)
3.1	-0.599 235 745 087 31(2)	9.5	-0.555 612 574 802 07(2)
3.2	-0.595 887 158 998 75(2)	10.0	-0.555 595 396 243 65(4)
3.3	-0.592 584 851 284 39(2)	11.0	-0.555 562 734 458 174 1(3)
3.4	-0.589 347 716 530 27(2)	12.0	-0.555 546 946 134 636 7(1)
3.5	-0.586 191 728 406 82(2)	13.0	-0.555 540 690 864 199(3)
3.6	-0.583 130 764 772 69(2)	14.0	-0.555 538 837 382 522(2)
3.7	-0.580 177 492 559 80(7)	15.0	-0.555 538 998 548 102 7(7)
3.8	-0.577 344 504 804 54(2)	16.0	-0.555 540 054 455 688 3(6)
3.9	-0.574 646 127 165 43(2)	17.0	-0.555 541 459 141 185(2)
4.0	-0.572 101 941 504 71(2)	18.0	-0.555 542 943 701 205 0(2)
4.1	-0.569 744 986 769 75(3)	19.0	-0.555 544 381 247 558 1(2)
4.2	-0.567 643 559 755 93(3)	20.0	-0.555 545 720 648 282 3(9)

Table S25: Calculated BO energies of the $6^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$6^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.202 641 598 69(2)	4.3	-0.560 674 017 760 1(3)
0.8	-0.324 500 922 089(5)	4.4	-0.559 945 453 737 23(2)
0.9	-0.410 295 909 591 1(3)	4.5	-0.559 001 202 875 92(3)
1.0	-0.471 816 865 441 68(2)	4.6	-0.557 725 475 834 69(5)
1.1	-0.516 448 097 681 65(4)	4.7	-0.556 395 851 361 61(8)
1.2	-0.549 016 995 231 0(3)	4.8	-0.555 152 589 518 86(3)
1.3	-0.572 789 910 477 8(2)	4.9	-0.554 047 866 481 40(4)
1.4	-0.590 040 231 465 7(4)	5.0	-0.553 087 437 035 14(4)
1.5	-0.602 387 943 182 67(4)	5.1	-0.552 248 891 677 81(5)
1.6	-0.611 010 642 495 95(3)	5.2	-0.551 499 832 906 54(5)
1.7	-0.616 779 044 647 38(2)	5.3	-0.550 814 472 452 66(5)
1.8	-0.620 346 479 277 93(3)	5.4	-0.550 180 840 970 31(5)
1.9	-0.622 209 453 218 48(8)	5.5	-0.549 598 863 602 96(4)
2.0	-0.622 749 514 292 36(3)	5.6	-0.549 074 754 670 68(4)
2.1	-0.622 262 736 930 76(3)	5.7	-0.548 615 994 494 34(3)
2.2	-0.620 980 838 141 68(4)	5.8	-0.548 228 289 617 1(3)
2.3	-0.619 086 526 355 1(2)	5.9	-0.547 914 216 636 9(3)
2.4	-0.616 724 808 602 68(2)	6.0	-0.547 672 880 172 1(2)
2.5	-0.614 011 421 770 9(5)	6.5	-0.547 335 908 502 23(2)
2.6	-0.611 039 189 061 81(5)	7.0	-0.547 650 550 036 9(2)
2.7	-0.607 882 860 873 8(4)	7.5	-0.547 897 320 962 16(4)
2.8	-0.604 602 836 083 84(2)	8.0	-0.547 913 907 956 75(2)
2.9	-0.601 248 047 933 25(3)	8.5	-0.547 790 806 336 19(2)
3.0	-0.597 858 221 180 43(3)	9.0	-0.547 660 594 840 44(2)
3.1	-0.594 465 652 863 831(5)	9.5	-0.547 617 955 732 00(2)
3.2	-0.591 096 630 815 79(2)	10.0	-0.547 711 312 331 50(2)
3.3	-0.587 772 577 493 95(5)	11.0	-0.548 337 384 286 99(1)
3.4	-0.584 510 989 231 73(3)	12.0	-0.549 411 024 800 08(2)
3.5	-0.581 326 232 121 50(2)	13.0	-0.550 662 304 409 24(2)
3.6	-0.578 230 258 089 34(2)	14.0	-0.551 858 357 462 26(4)
3.7	-0.575 233 333 286 372(2)	15.0	-0.552 873 467 879 47(2)
3.8	-0.572 344 913 219 41(2)	16.0	-0.553 672 028 175 34(5)
3.9	-0.569 575 185 579 46(3)	17.0	-0.554 268 597 452 81(2)
4.0	-0.566 938 484 523 47(2)	18.0	-0.554 697 647 730 37(4)
4.1	-0.564 464 419 719 30(3)	19.0	-0.554 996 982 396 59(2)
4.2	-0.562 247 948 033 40(7)	20.0	-0.555 200 395 566 37(3)

Table S26: Calculated BO energies of the $7^3\Sigma_u^+$ state in atomic units (hartree). Uncertainties originate purely from extrapolation to CBS limit.

$7^3\Sigma_u^+$			
R/au	E/au	R/au	E/au
0.7	-0.197 341 162 11(6)	4.3	-0.558 292 990 692(2)
0.8	-0.319 338 039 10(5)	4.4	-0.556 768 762 632 0(9)
0.9	-0.405 281 585 88(3)	4.5	-0.554 952 260 223(2)
1.0	-0.466 957 462 89(4)	4.6	-0.553 189 345 326 9(10)
1.1	-0.511 744 599 48(3)	4.7	-0.551 586 044 062(4)
1.2	-0.544 465 066 29(3)	4.8	-0.550 190 627 456(5)
1.3	-0.568 380 724 75(4)	4.9	-0.549 007 351 538(6)
1.4	-0.585 761 774 52(2)	5.0	-0.547 986 124 77(4)
1.5	-0.598 226 412 81(2)	5.1	-0.547 057 231 855(5)
1.6	-0.606 951 658 76(2)	5.2	-0.546 175 316 319(4)
1.7	-0.612 808 536 545(7)	5.3	-0.545 323 938 182(4)
1.8	-0.616 451 243 723(6)	5.4	-0.544 500 389 588 13(7)
1.9	-0.618 377 448 729(4)	5.5	-0.543 704 927 945 25(10)
2.0	-0.618 969 968 931(3)	5.6	-0.542 937 289 953 19(2)
2.1	-0.618 526 140 451(7)	5.7	-0.542 196 645 715 466(5)
2.2	-0.617 278 870 265(3)	5.8	-0.541 482 275 985 524(4)
2.3	-0.615 411 955 804(2)	5.9	-0.540 793 973 238 49(2)
2.4	-0.613 071 384 23(9)	6.0	-0.540 132 059 317 39(3)
2.5	-0.610 373 767 958 8(9)	6.5	-0.537 241 910 057 52(7)
2.6	-0.607 412 712 187(4)	7.0	-0.535 077 096 536 0(6)
2.7	-0.604 263 669 798 6(8)	7.5	-0.533 589 160 715 0(2)
2.8	-0.600 987 678 564 9(7)	8.0	-0.532 667 015 481 8(3)
2.9	-0.597 634 264 025 8(8)	8.5	-0.532 224 049 302 2(5)
3.0	-0.594 243 715 258 6(9)	9.0	-0.532 157 563 605 9(8)
3.1	-0.590 848 887 294 4(6)	9.5	-0.532 189 830 368 0(5)
3.2	-0.587 476 647 141 1(3)	10.0	-0.532 231 760 266 8(4)
3.3	-0.584 149 056 339(2)	11.0	-0.532 267 938 149 0(2)
3.4	-0.580 884 370 693 1(2)	12.0	-0.532 214 223 673 4(2)
3.5	-0.577 697 940 323 6(6)	13.0	-0.532 085 449 987 47(8)
3.6	-0.574 603 123 013 8(2)	14.0	-0.531 920 294 357 51(7)
3.7	-0.571 612 420 141 0(2)	15.0	-0.531 756 774 057 73(7)
3.8	-0.568 739 337 874 6(2)	16.0	-0.531 617 944 617 63(7)
3.9	-0.566 002 457 570 4(2)	17.0	-0.531 511 015 390 29(6)
4.0	-0.563 437 024 798 3(6)	18.0	-0.531 433 363 736 03(5)
4.1	-0.561 136 404 454 3(2)	19.0	-0.531 378 733 810 95(4)
4.2	-0.559 385 126 958 3(3)	20.0	-0.531 340 828 453 86(4)